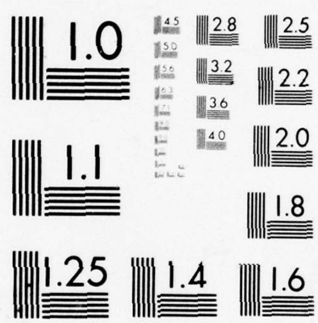
AD-A053 491 PRINCETON UNIV N J DEPT OF CHEMISTRY F/G 7/3
REACTIONS OF TRANSITION METAL NITROGEN SIGMA-BONDS. 5. CARBONAT--ETC(U)
APR 78 M H CHISHOLM, F A COTTON, M W EXTINE N00014-76-C-0826
UNCLASSIFIED TR-78-11 NL

1 OF 1
AD
A053491

END
DATE
FILMED
6-78
DDC



MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

(12)

AD A053491

AD No. ____
DDC FILE COPY

OFFICE OF NAVAL RESEARCH

Contract N00014-76-C-0826

Task No. NR 056-625

TECHNICAL REPORT NO. 78-11

Reactions of Transition Metal Nitrogen σ-Bonds. 5 Carbonation of Tetrakisdiethylamido Chromium(IV) to Yield Binuclear Chromium(III) and -(II) Carbamato Complexes.

by M. H. Chisholm,[1] F. A. Cotton,[2] M. W. Extine[2]

and D. C. Rideout[1]

Departments of Chemistry

[1]Princeton University

Princeton, New Jersey 08540

and

[2]Texas A & M University

College Station. Texas 77843

Prepared for Publication

in

Inorganic Chemistry

April 20, 1978

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE

READ INSTRUCTIONS BEFORE COMPLETING FORM

1. REPORT NUMBER sigma

2. GOVT ACCESSION NO.

3. RECIPIENT'S CATALOG NUMBER

4. TITLE (and Subtitle) Reactions of Transition Metal Nitrogen σ-Bonds. 5. Carbonation of Tetrakisdiethylamido Chromium(IV) to Yield Binuclear Chromium(III) and -(II) Carbamato Complexes.

5. TYPE OF REPORT & PERIOD COVERED Technical Report, 1978

6. PERFORMING ORG. REPORT NUMBER TR-78-11

7. AUTHOR(s) M. H. Chisholm, F. A. Cotton, M. W. Extine and D. C. Rideout

8. CONTRACT OR GRANT NUMBER(s) N00014-76-C-0826, NR 056-625

9. PERFORMING ORGANIZATION NAME AND ADDRESS
Department of Chemistry
Princeton University
Princeton, N. J. 08540

10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS 20 Apr 78

11. CONTROLLING OFFICE NAME AND ADDRESS
Office of Naval Research
Department of the Navy

12. REPORT DATE April 20, 1978

13. NUMBER OF PAGES 47

14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)

15. SECURITY CLASS. (of this report) 50p

15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Metal-Nitrogen Bonds, Carbon Dioxide, Insertion, Chromium.

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

From the reaction between Cr(NEt)$_4$ and CO_2 (4 equiv) two crystalline compounds have been isolated and structurally characterized: I, $Cr_2(O_2CNEt_2)_4(\mu\text{-}NEt_2)_2$ and II, $Cr_2(O_2CNEt_2)_4 2HNEt_2$. Compound I is the major product when CO_2 is allowed to react slowly with $Cr(NEt_2)_4$; compound II predominates when CO_2 (4 equiv) is added rapidly. These results are compared with previous studies of CO_2 insertion reactions involving early transition metal dialkylamides and with the known reactions of $Cr(NEt_2)_4$. A reaction pathway leading from

DD FORM 1473, 1 JAN 73 — EDITION OF 1 NOV 65 IS OBSOLETE

S/N 0102-LF-014-6601

Unclassified

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

400 363

beta

$Cr(NEt_2)_4$ to I and II is proposed to involve β-hydrogen elimination from a $[Cr^{IV}-NEt_2]$ moiety followed by reductive elimination of Et_2NH and the generation of Cr(II).

I crystallizes in space group Pbcn with a = 19.122(8), b = 11.024(2), c = 18.114(6)Å, V = 3818(3)$Å^3$, and Z = 4. The structure was solved and refined to yield R_1 = 0.082 and R_2 = 0.109. I has crystallographic C_2 symmetry and consists of two distorted edge-sharing octahedra with bridging diethylamido groups. The $Cr_2N_2(O-O)_4$ moiety has virtual D_2 symmetry. Important distances are Cr-Cr = 2.948(2) and Cr-N (av) = 2.046Å; average Cr-O distances trans to N are 2.065Å while Cr-O distances cis to N are 1.996Å. II crystalizes in the space group P$\bar{1}$ with a = 10.936(2), b = 11.170(2), c = 8.871(2)Å, α = 99.46(1), β = 98.56(1), γ = 108.58(1)°, V = 989.4(6)$Å^3$, and Z = 2. The structure was solved and refined to yield R_1 = 0.071 and R_2 = 0.098. The molecule adopts the classical dichromium tetracarboxylato-tupe structure with axial (Cr-Cr-N = 178.1(3)°) diethylamine ligands. II has imposed C_i symmetry with the $Cr_2O_8N_2$ core having near D_{4h} symmetry; Cr-Cr = 2.384(2)Å, Cr-N = 2.452(8), and average Cr-O = 2.018(7)Å.

beta

gamma

alpha

ACCESSION for		
NTIS	White Section	☑
DDC	Buff Section	☐
UNANNOUNCED		☐
JUSTIFICATION		
BY		
DISTRIBUTION/AVAILABILITY CODES		
Dist.	AVAIL. and/or SPECIAL	
A		

S/N 0102-LF-014-6601

Submitted to

Contribution from Departments of Chemistry,
Texas A&M University, College Station, Texas 77843
and Princeton University, Princeton, N. J. 08540

REACTIONS OF TRANSITION METAL NITROGEN σ-BONDS. 5[1]

CARBONATION OF TETRAKISDIETHYLAMIDO CHROMIUM(IV) TO YIELD BINUCLEAR CHROMIUM(III) AND -(II) CARBAMATO COMPLEXES

by M. H. Chisholm,[2a*] F. A. Cotton,[2b*] M. W. Extine[2b] and D. C. Rideout[2a]

ABSTRACT

From the reaction between $Cr(NEt)_4$ and CO_2 (4 equiv) two crystalline compounds have been isolated and structurally characterized: I, $Cr_2(O_2CNEt_2)_4$-$(\mu\text{-}NEt_2)_2$ and II, $Cr_2(O_2CNEt_2)_4 2HNEt_2$. Compound I is the major product when CO_2 is allowed to react slowly with $Cr(NEt_2)_4$; compound II predominates when CO_2 (4 equiv) is added rapidly. These results are compared with previous studies of CO_2 insertion reactions involving early transition metal dialkylamides and with the known reactions of $Cr(NEt_2)_4$. A reaction pathway leading from $Cr(NEt_2)_4$ to I and II is proposed to involve β-hydrogen elimination from a $[Cr^{IV}\text{-}NEt_2]$ moiety followed by reductive elimination of Et_2NH and the generation of Cr(II).

I crystallizes in space group Pbcn with a = 19.122(8), b = 11.024(2), c = 18.114(6)Å, V = 3818(3)Å^3, and Z = 4. The structure was solved and refined to yield R_1 = 0.082 and R_2 = 0.109. I has crystallographic C_2 symmetry and consists of two distorted edge-sharing octahedra with bridging diethylamido groups. The $Cr_2N_2(O\text{-}O)_4$ moiety has virtual D_2 symmetry. Important distances are Cr-Cr = 2.948(2) and Cr-N (av) = 2.046Å; average Cr-O distances trans to N are 2.065Å while Cr-O distances cis to N are 1.996Å. II crystalizes in the space group P$\bar{1}$ with a = 10.936(2), b = 11.170(2), c = 8.871(2)Å, α= 99.46(1), β = 98.56(1), γ = 108.58(1)°, V = 989.4(6)Å^3, and Z = 2. The structure was

solved and refined to yield $R_1 = 0.071$ and $R_2 = 0.098$. The molecule adopts the classical dichromium tetracarboxylato-type structure with axial (Cr-Cr-N = 178.1(3)°) diethylamine ligands. II has imposed C_i symmetry with the $Cr_2O_8N_2$ core having near D_{4h} symmetry; Cr-Cr = 2.384(2)Å, Cr-N = 2.452(8), and average Cr-O = 2.018(7)Å.

INTRODUCTION

It is characteristic of early transition metal dialkylamides, $M_m(NR_2)_n$, that they react readily in solution with carbon dioxide to yield complexes containing the carbamato anion, $R_2NCO_2^-$, as a ligand.[1] In some cases, mononuclear dialkylamides react to convert all R_2N groups to R_2NCO_2, as in (1), while for $W(NMe_2)_6$ only

$$M(NMe_2)_n + nCO_2 \rightarrow M(O_2CNMe_2)_n \qquad (1)$$

$$M = Ti,\ V,\ Zr;\ n = 4$$

$$M = Nb,\ Ta;\ n = 5$$

$W(NMe_2)_3(O_2CNMe_2)_3$ can be obtained even in the presence of excess CO_2. However, even in cases where fully carbonated products are obtainable, the use of <n equiv. CO_2 allows the isolation of partly carbonated compounds such as $Ti(NMe_2)_2(O_2CNMe_2)_2$, $Ti(NMe_2)(O_2CNMe_2)_3$ and $Ta(NMe_2)_2(O_2CNMe_2)_3$.[1,3]

Similarly, several dinuclear, triply-bonded dialkylamides react readily with CO_2. $W_2(NMe_2)_6$ and $W_2(NEt_2)_4Me_2$ have yielded, respectively, $W_2(O_2CNMe_2)_6$ and $W_2(O_2CNEt_2)_4Me_2$.[4]

All of these, and other, carbonation reactions have proceeded rapidly, essentially quantitatively and without any observed changes in oxidation numbers, of the sort found when CS_2 is inserted, e. g.,[5,6]

$$W(NMe_2)_6 + 6\ CS_2 \longrightarrow W(S_2CNMe_2)_4 + (Me_2NC(S)S-)_2$$

$$Nb(NMe_2)_5 + 5\ CS_2 \longrightarrow Nb(S_2CNMe_2)_4 + 1/2(Me_2NC(S)S-)_2$$

Also, there has been no prior example of the conversion of a mononuclear metal dialkylamide to a binuclear carbamato product.

We report here the occurrence of an unprecedented type of reaction, in which both of the aforementioned processes take place when $Cr(NEt_2)_4$ reacts

with an excess of CO_2. The reaction is complex and yields products in proportions depending sensitively upon reaction conditions. One compound which has not been detected is the "obvious" product, $Cr(O_2CNEt_2)_4$. We also show conclusively, by x-ray crystallography, the identity and structures of two of the products, $Cr_2(O_2CNEt_2)_4(\mu\text{-}NEt_2)_2$, I, a binuclear chromium(III) complex, and $Cr_2(O_2CNEt_2)_4 \cdot 2HNEt_2$, II, a quadruply-bonded dichromium(II) complex in which bridging carbamato groups are observed for the first time in any quadruply-bonded M_2 compound.

EXPERIMENTAL

General procedures and physical instrumentation were as previously described.[1] $Cr(NEt_2)_4$ was prepared by a modification of the published procedure.[7] Diethyl ether/hexane solvent mixture was used for the reaction between $CrCl_3$ and $LiNEt_2$ (3 equiv).

Preparation of Bis(diethylamido)tetrakis(diethylcarbamato)dichromium(III).

$Cr(NEt_2)_4$(5.78 mmol) in hexanes (180mL) was exposed to CO_2(25 mmol) in a calibrated vacuum manifold at room temperature. An immediate uptake of CO_2 was noted by a reduction in CO_2 pressure. After 10 min. the remaining CO_2 was condensed into the reaction flask at -196°C. The reaction mixture was then allowed to warm to room temperature and was stirred magnetically for 10 h. A fine pale blue-green precipitate was removed by filtration and the filtrate, which appeared dark green under fluorescent lighting and red in incandescent light, was reduced in volume to 120 mL and cooled -20°C for 10 h yielding dark green crystals of $Cr_2(O_2CNEt_2)_4(\mu\text{-}NEt_2)_2$ which were collected and dried under vacuum (25°, 10^{-2} Torr): 0.738g, 36% yield based on Cr. Analysis Found (Calcd) for $C_{28}H_{60}N_6O_8Cr_2$: C, 46.77(47.18); H, 7.99(8.45); N, 11.02(11.79).

IR data obtained from a nujol mull between CsI plates in the region 1500-200 cm^{-1} 1485(s), 1378(s), 1337(m), 1322(s), 1262(w), 1209(m), 1133(w), 1112(m), 1099(m), 1090(m), 1083(m), 1075(m), 1040(w), 1007(w), 977(w), (37(w), 896(w), 836(s), 790(s, br), 641(s, br), 610(s), 572(w), 495(s), 482(m), 461(m), 495(s), 482(m), 460(m), 421(m), 402(m), 348(m, br), 263(w).

Mass spectral data obtained by direct insertion at 100°C: $m/_e$ = 712 $[Cr_2(O_2CNEt_2)_4(NEt_2)_2]^+$ small; $m/_e$ = 641 $[Cr_2(O_2CNEt_2)_4(HNEt_2)]^+$ medium, $m/_e$ = 640 $[Cr_2(O_2CNEt_2)_4NEt_2]^+$ base peak; $m/_e$ - 596 $[Cr_2(O_2CNEt_2)_3(NEt_2)_2]^+$ small; $m/_e$ = 563, large; $m/_e$ = 452 $[Cr_2(O_2CNEt_2)_2(NEt_2)(HNEt)]^+$ medium; $m/_e$ = 356 $[Cr(O_2CNEt_2)_2NEt_2]^+$ large. Magnetic Susceptibility Data obtained from toluene solution by the method of D. F. Evans (J. Chem. Soc. 2003 (1959.):

μ_{eff} per Cr atom in B.M. (Temperature in °K): 2.25 (355°); 2.15 (310°); 2.09(283°); 2.00(251°); 1.86(218°); 1.78(210°).

Reaction of $Cr_2(O_2CNEt_2)_4(NEt_2)_2$ with Excess CO_2.

CO_2 (3 mmol) was added to a frozen solution of $Cr_2(O_2CNEt_2)_4(NEt_2)_2$ (0.205 mmol) in toluene (10mL) at -196°C. The flask was warmed to room temperature and the solution was stirred for 13 h. The solvent was stripped yielding a dark green solid which was identified as the starting material by i.r. spectroscopy.

Preparation of Bis(diethylamine)tetrakis(diethylcarbamato)dichromium(II).

CO_2(15.33 mmol) was added to a frozen solution (-196°C) of $Cr(NEt_2)_4$ (3.41 mmol) in hexane (50mL). The closed system was allowed to warm to room temperature and stirred magnetically for 10 h. The resulting red solution contained a small amount of a pale blue-green precipitate which was removed by filtration. The filtrate was stripped to dryness and the residue was

redissolved in hexane at ca. 60°C and then cooled to ca. -20°C yielding reddish-orange crystals of $Cr_2(O_2NEt_2)_4(HNEt_2)_2$. Analysis Found (Calcd) for $C_{28}H_{62}N_6O_8Cr_2$: C, 47.01(47.04); H, 8.66(8.74); N, 11.61(11.70).

I.r. data obtained from a nujol mull between CsI plates (1500-200 cm^{-1}). 1346(s), 1330(m), 1310(w), 1271(m), 1242(w), 1188(s), 1145(s), 1085(m), 1067(s), 1047(s), 996(vs, br), 914(m), 887(m), 869(vs), 788(vs, br), 596(s), 589(s), 537(s), 509(m), 348(vs), 328(m), 316(m), 297(m), 230(w). ^{1}HNMR (benzene-d_6, 30°C) δ=2.10-5.90(br, CH_2), δ=1.33(t, J=6Hz, CH_3): the compound is apparently slightly paramagnetic.

<u>Organic Volatiles formed in the Reaction between $Cr(NEt_2)_4$ and CO_2.</u>

A 50mL round bottomed flask containing neat $Cr(NEt_2)_4$(3.47mmol) was rotated to coat its walls with the dark green liquid. The flask was then attached to a vacuum manifold and, by cooling to -196°C, CO_2 (10.4mmol) was added. The system was allowed to warm to room temperature and with the use of a heat gun all the volatiles were collected in an NMR tube containing toluene-d_8 frozen at -196°C. The tube was then sealed with a torch. ^{1}H nmr spectroscopy revealed the presence of diethylamine and N-ethylididene-ethylamine in approximately equal quantities. The ^{1}H nmr data obtained at 30°, from toluene-d_8 at 60MHz for $CH_3CH_2N{=}CHCH_3$ were δ=7.40(m, broad, = CH), δ=3.25(q, J=7.9, CH_2), δ=1.70(dt, J=4.9, J_2=1.1, $\underline{CH_3}CH{=}N{-}CH_2$), δ=1.12(t, J=7.0, $\underline{CH_3}CH_2{-}N$) which may be compared to the reported ^{1}H nmr data of $CH_3CH{=}NCH_3$: δ=7.67(q.q, J_1=4.8, J_2=1.8 N=CH-), δ=3.23(dq, J_1=1.8, J_2=1.4, $\underline{CH_3}{-}N$), δ=1.92(dq, J_1=4.8, J_2=1.4 $N{=}CH\underline{CH_3}$). δ are in ppm rel. TMS and J values are in Hz.

<u>Crystallographic Study of I.</u>[8] Crystals were mounted by wedging them in mineral oil filled, thin-walled capillaries, and several were examined before one of good quality was found, measuring 0.20 x 0.25 x 0.35 mm. ω-scans of several intense reflections had peak widths at half-height of *ca*. 0.2°. Preliminary lattice constants and axial photographs indicated that the crystal belonged to the orthorhombic system. The final lattice constants, determined at 3°C from the setting angle of 15 reflections in the range, $23° < 2\theta(\mathrm{CuK}\alpha) < 38°$, chosen to give a good sampling of diffractomater settings and indices are a = 19.122(8), b = 11.024(2), c = 18.114(6)Å, and V = 3818(2)$Å^3$. The observed volume was consistent with that expected for Z = 4. The systematic absences observed during data collection, $0k\ell$ ($k = 2n+1$), $k0\ell$ ($\ell = 2n+1$), and $hk0$ ($h+k = 2n+1$), uniquely determined the space group to be Pbcn (No. 60).

The data were collected using Cu Kα (λ = 1.54184Å) radiation at 3°C with a Syntex P$\bar{1}$ autodiffractometer (located in a cold room maintained at 3±1°) equipped with a graphite crystal monochromator. Variable scan rates from 4.0 to 24.0°/min were used for symmetric θ/2θ scans ranging from 1.0° below to 1.0° above the calculated Cu $K\alpha_1$-$K\alpha_2$ doublet. A total of 3157 unique reflections having $0° < 2\theta\mathrm{CuK}\alpha < 120°$ were recorded. The ratio of background to scan time was 0.5. The intensities of three standard reflections were monitored frequently throughout data collection and showed no decrease in intensity. The data were reduced to a set of relative $|F_o|^2$ values. The intensities were corrected for absorption effects (μ = 53.3 cm^{-1}); transmission coefficients ranged from 0.325 to 0.433 with an average of 0.386. The 1512 reflections having $|F_o|^2 > 3\sigma(|F_o|^2)$ were retained as observed and used in subsequent structure solution and refinement. The positions of the 22 unique non-hydrogen atoms were determined using standard heavy atom methods, i.e., a Patterson solution,

followed by several rounds of least squares refinement and difference Fouier syntheses. Positional and isotropic thermal parameters of the 25 non-hydrogen atoms were refined in several least squares cycles to yield discrepancy indices

$$R_1 = \Sigma||F_o|-|F_c||/|F_o| = 0.087$$
$$R_2 = (\Sigma w||F_o|-|F_c||^2/\Sigma w|F_o|^2)^{1/2} = 0.114$$

The structure was refined to convergence using anisotropic thermal parameters for the Cr, O, and N atoms and isotropic thermal parameters for the C atoms. The final discrepancy indices were $R_1 = 0.082$ and $R_2 = 0.109$. The estimated standard deviation of an observation of unit weight was 2.11. A final difference Fourier map showed no features of structural significance.

Crystallographic Study of II.[8] A crystal measuring *ca*. 0.25 x 0.4 x 0.4 mm was mounted, embedded in epoxy, in a thin-walled glass capillary. Omega scans of several intense low-angle reflections had peak widths at half-height of 0.2°. Cell constants and axial photographs indicated that the crystal belonged to the triclinic system. Cell constants, determined at 23°C using MoKα (λ = 0.710730Å) radiation, are a = 10.936(2), b = 11.170(2), c = 8.871(2)Å, α = 99.46(1), β = 98.56(1), γ = 108.58°, V = 989.4(7)Å^3. The observed volume was consistent with that expected for Z = 1.

The data were collected at 23°C using a Syntex P$\bar{1}$ autodiffractometer and graphite crystal monochromatized MoKα (λ = 0.710730Å) radiation. Otherwise, data were collected as for I (see above). A total of 2600 unique reflections having $0° < 2\theta(\text{MoK}\alpha) \leq 45.00°$ were collected. The intensities of three standard reflections were monitored frequently and showed no decrease over the period of data collection. The data were reduced to a set of relative $|F_o|^2$ values and the 1565 observations having $|F_o|^2 > 3\sigma(|F_o|^2)$ were used in subsequent structure solution and refinement. Data were not corrected for absorption (μ = 6cm^{-1}).

The space group was assumed to be $P\bar{1}$ (No. 2) and this was verified by the successful structure solution and refinement. The structure was solved by conventional heavy atom methods.

The terminal diethylamino ligand is disordered with the methylene carbon atoms assumed to be distributed equally over two positions whilst the nitrogen atom and methyl groups are in the same positions for both orientations. The structure was refined to convergence using anisotropic thermal parameters for all non-hydrogen atoms except the carbon atoms in the axial $HNEt_2$ ligands.

Final unweighted and weighted residuals were 0.071 and 0.098, respectively. The esd of an observation weight was 2.07. A value of 0.07 was used for P in the calculation of the weights. The largest peaks in the final difference Fourier map were in the region of the disordered axial ligands, presumably because of the anisotropic motion of the alkyl groups and additional disorder.

Tables of observed and calculated structure factors for both structures (14 pages) are available as supplementary material. See any current masthead page for ordering information.

RESULTS AND DISCUSSION

Synthesis. Hydrocarbon solutions of $Cr(NEt_2)_4$ react rapidly with CO_2, even at $-78^{\circ}C$. In procedure 1 (see experimental section) the hydrocarbon solution of $Cr(NEt_2)_4$ is initially allowed to react slowly at room temperature with CO_2. Here the major chromium containing species formed is a dark-green, hydrocarbon soluble, crystalline compound $Cr_2(O_2CNEt_2)_4(\mu\text{-}NEt_2)_2$, I. Compound I is inert to further reaction with CO_2 under these conditions. In procedure 2 the reaction is carried out by condensing CO_2(> 4 equiv) into a reaction flask containing the hydrocarbon solution of $Cr(NEt_2)_4$ cooled below $-78^{\circ}C$. The sealed system is then allowed to

warm to room temperature. Here an initial rapid reaction occurs and the major chromium containing product is a red, crystalline, hydrocarbon-soluble compound $Cr_2(O_2CNEt_2)_4(HNEt_2)_2$,II. In both reaction procedures I and II are formed competitively along with another compound which is a pale-blue-green, hydrocarbon insoluble powder. The latter is a minor product and is believed to be polymeric $Cr(O_2CNEt_2)_3$. The only volatile organic species formed in these reactions are Et_2NH and EtN=CHMe.

DISCUSSION

Aside from polymeric CrF_4, the only well known compounds of quadrivalent chromium are CrL_4 compounds, where L = a β-elimination stabilized alkyl, a dialkylamido or a tertiary alkoxy ligand.[9] In this CrL_4 series chromium is always four-coordinate. All previous attempts to extend the CrL_4 series to give higher coordination numbers failed and products of trivalent chromium were obtained e.g. as in reactions 1 and 2 below.

1[7] $2Cr(NEt_2)_4 + 8CS_2 \rightarrow 2Cr(S_2CNEt_2)_3 + (Et_2NC(S)S-)_2$

2[7,10] $2Cr(NEt_2)_4 + 7RR'CHOH \rightarrow 2Cr(OCHRR')_3 + 8HNEt_2 + RR'C{=}O$

where R, R' = alkyl or H.

The formation of trivalent chromium in the reaction between $Cr(NEt_2)_4$ and CO_2 is therefore not surprising, but the formation of divalent chromium products is most unexpected.

A plausible reaction pathway leading to the compound in Scheme 1. Our proposal is that CO_2 insertion into a Cr-N bond of $Cr^{IV}(NEt_2)_4$ promotes β-hydrogen elimination from a coordinated diethylamido ligand and then by reductive elimination of Et_2NH, a reactive divalent chromium species, $Cr^{II}(O_2CNEt_2)(NEt_2)$, is formed.[11] The subsequent reaction pathway is dependent on the relative concentration of CO_2. At low concentrations of CO_2, a reaction between $Cr^{II}(O_2CNEt_2)(NEt_2)$ and $Cr^{IV}(NEt_2)_4$ will lead to dimeric Cr(III) compounds and ultimately to I. At initial high CO_2 concentrations divalent chromium will

predominate and thus II will be the dominant product. Since the mechanism for CO_2 insertion into a M-NR_2 group involves electrophilic attack on the nitrogen lone pair the bridging diethylamido ligands in I, which have quaternized nitrogens, are inert to further attack by CO_2.

Structural. Atomic parameters for $Cr_2(O_2CNEt_2)_4(NEt_2)_2$, I, and $Cr_2(O_2CNEt_2)_4(NHEt_2)_2$, II are presented in Tables I and II, respectively. ORTEP views of I and II depicting the atom labelling schemes are shown in Figures 1 and 3. Figure 2 shows a stereoview of I.

Compound I crystallizes in discrete dinuclear molecules in the orthorhombic space group Pbcn with Z = 4. Each molecule has crystallographic C_2 symmetry with the twofold axis bisecting the Cr-Cr' and N(1)-N(1)' vectors. The interatomic distances and angles are listed in Table III. The $Cr_2O_8N_2$ moiety has virtual D_2 symmetry and can be described as two octahedra sharing an edge. Each molecule is chiral and there are two molecules of each enantiomorph in the unit cell, those of opposite hand related by the inversion centers and those of the same hand related by the screw axes.

The "octahedral" coordination about the chromium atoms is, of course, distorted by the short "bite" of the bidentate carbamato ligands which is only 2.178(6)Å whereas an edge of the coordination octahedron should be ca. 2.87Å. The bidentate ligands are evidently spanning edges of the idealized octahedra since the angles between the N(1)/Cr/N(1)', O(1)/Cr/O(2) and O(3)/Cr/O(4) planes range from 85 to 95°. As expected, each of the CrO_2CNC_2 moieties is essentially planar, as is the central Cr_2N_2 moiety. The diethylamido groups symmetrically bridge the chromium atoms, while the bidentate carbamato ligands are bonded slightly assymetrically. The two Cr-O distances (2.066(5) and 2.063(5)Å) which are "trans" to nitrogen (N-Cr-O = 164°) are 0.074Å longer than the Cr-O distances (1.993(4) and 1.988(5)Å) which are "cis"(O-Cr-N = 98°) to nitrogen. This type of trans effect has been noted previously in mononuclear $M(NMe_2)_m$-$(O_2CNMe_2)_n$ compounds.[1,3]

The long Cr-Cr distance of 2.948(2)Å is consistent with the conclusion that no significant Cr-Cr bonding interaction exists. The compound is paramagnetic and shows strong antiferomagnetic coupling as evidenced by the marked reduction in μ_{eff} from the spin only value and the temperature dependent properties of μ_{eff}. It is particularly interesting to note that the closely related molybdenum compound $Mo_2(NMe_2)_2(O_2CNMe_2)_4$[12a] is diamagnetic and believed to contain a Mo-to-Mo triple bond with a structure akin to that found for $W_2Me_2(O_2CNEt_2)_4$.[12b] This provides a good example of how for the group VI metals in their trivalent state metal-to-metal bonding increases down the series c.f. the $M_2Cl_9{}^{3-}$ ions which have the confacial bioctahedron structure where the metal-to-metal distances are 3.12, 2.67 and 2.45Å for Cr, Mo and W respectively.[13]

Compound II crystallizes in discrete dinuclear molecules in the triclinic space group $P\bar{1}$ with Z = 1, and the molecule has crystallographically imposed C_i symmetry. Table IV lists bond lengths and angles. The compound has four bridging carbamato ligands and two axially coordinated molecules of diethylamine. This type of structure, $Cr(O\text{-}O)_4L_2$, is typical of dichromium tetracarboxylates. The $Cr_2O_8N_2$ core has essential D_{4h} symmetry. The average Cr-O distance of 2.018(7)Å is in the range found for $Cr_2(O_2CR)_4L_2$ compounds.

The rough inverse correlation between Cr-Cr distances and Cr-L axial distances has been noted for $Cr_2(O_2CR)_4L_2$ compounds.[14] The Cr-Cr distance we find for II is somewhat longer than might be expected from the axial Cr-N distance of 2.452(8)Å. The point for this compound is, in fact, close to that for $Cr_2(O_2CCMe_3)_4$ and both lie well away from the region expected on the basis of the structure for about a dozen other compounds. The fact that the axial donor here is an aliphatic amine nitrogen atom may be one cause of the unexpectedly long Cr-Cr bond, but perhaps the only safe comment is that this structure provides further evidence that length of a Cr-Cr quadruple bond is extremely sensitive to the properties of the ligands surrounding it.

Acknowledgements. This work was supported by the National Science Foundation at Texas A&M University and by the Office of Naval Research at Princeton University.

Scheme 1

$$Cr^{IV}(NEt_2)_4 + CO_2 \rightarrow Cr^{(IV)}(NEt_2)_3(O_2CNEt_2)$$

$$\Big\downarrow \text{β-hydrogen elimination}$$

$$(EtN{=}CHMe)Cr^{IV}(H)(NEt_2)_2(O_2CNEt_2)$$

$$\Big\downarrow -Et_2NH, EtN{=}CHMe$$

$$I \xleftarrow{CO_2} Cr_2^{III}(NEt_2)_5(O_2CNEt_2) \xleftarrow{+Cr^{IV}(NEt_2)_4} Cr^{II}(NEt_2)(O_2CNEt_2)$$

$$\Big\downarrow + CO_2$$

$$I \xleftarrow{CO_2} Cr_2^{III}(NEt_2)_4(O_2CNEt_2)_2 \xleftarrow{Cr^{IV}(NEt_2)_4} Cr^{II}(O_2CNEt_2)_2$$

$$\Big\downarrow + Cr^{II},\ + Et_2NH.$$

$$II$$

REFERENCES

1. Part 3 and 4: (a) M. H. Chisholm and M. W. Extine, J. Amer. Chem. Soc., 99, 782 (1977); (b) ibid., 99, 792 (1977).

2. (a) Princeton University; (b) Texas A&M University.

3. M. H. Chisholm, F. A. Cotton and M. W. Extine, Inorg. Chem., 17, xxxx (1978).

4. M. H. Chisholm, F. A. Cotton, M. W. Extine, and B. R. Stults, Inorg. Chem., 16, 603 (1977).

5. D. C. Bradley, M. H. Chisholm, M. W. Extine, and M. E. Stager, Inorg. Chem., 16, 1794 (1977).

6. D. C. Bradley and M. H. Gitlitz, J. Chem. Soc., A, 1152 (1969).

7. J. S. Basi, D. C. Bradley and M. H. Chisholm, J. Chem. Soc., A, 1433 (1971).

8. All crystallographic computing was carried out on a PDP 11/45 computer owned by Molecular Structure Corporation, College Station, Texas, using the Enraf-Nonius Structure Determination Package.

9. ref. 10. p. 840 and references cited therein.

10. E. C. Alyea, J. S. Basi, D. C. Bradley and M. H. Chisholm, J. Chem. Soc., A, 772 (1971).

11. A radical pathway leading to Cr(III) products and Et_2NH and EtN=CHMe could be proposed akin to that for that found for reaction 2 (ref. 7013). However, this would not account for the formation of Cr(II) compounds.

12. (a) M. H. Chisholm and W. W. Reichert, Inorg. Chem., 17, 767 (1978); (b) M. H. Chisholm, F. A. Cotton, M. W. Extine and B. R. Stults, Inorg. Chem., 16, 603 (1977).

13. See F. A. Cotton and G. Wilkinson in "Advanced Inorganic Chemistry", Interscience Publisher, New York and London 1072, 3rd Ed., p. 961 and references cited therein.

14. F. A. Cotton, M. W. Extine, and G. W. Rice, Inorg. Chem., 17, 176 (1978); F. A. Cotton and G. W. Rice, Inorg. Chem., 17, xxx (1978).

Table I. POSITIONAL AND THERMAL PARAMETERS AND THEIR ESTIMATED STANDARD DEVIATIONS for $Cr_2(O_2CNEt_2)_4(NEt_2)_2$.[a]

Atom	X	Y	Z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Cr	0.07640(8)	0.1488(1)	0.23926(8)	0.00261(4)	0.0070(1)	0.00259(4)	-0.0003(2)	0.00006(9)	0.0003(2)
O(1)	0.0967(3)	0.3261(5)	0.2406(4)	0.0031(2)	0.0074(6)	0.0036(2)	-0.0001(6)	-0.0006(4)	0.0006(6)
O(2)	0.1641(3)	0.1984(6)	0.2987(4)	0.0029(2)	0.0083(6)	0.0033(2)	-0.0003(6)	-0.0000(4)	0.0007(7)
O(3)	0.0950(3)	-0.0284(6)	0.2342(3)	0.0034(2)	0.0089(6)	0.0030(2)	0.0001(6)	0.0005(4)	0.0013(6)
O(4)	0.1442(3)	0.0960(6)	0.1567(4)	0.0031(2)	0.0075(6)	0.0033(2)	0.0008(7)	0.0013(4)	0.0005(6)
N(1)	0.0097(4)	0.1501(7)	0.3276(4)	0.0029(2)	0.0082(7)	0.0024(2)	-0.0000(9)	-0.0003(4)	-0.0000(8)
N(2)	0.1883(5)	0.4012(7)	0.3076(5)	0.0037(3)	0.0093(8)	0.0037(3)	-0.0028(9)	-0.0001(5)	-0.0001(9)
N(3)	0.1644(5)	-0.1066(7)	0.1434(4)	0.0049(3)	0.0080(8)	0.0031(3)	0.0030(9)	0.0014(6)	0.0001(8)
C(1)	0.0177(5)	0.0376(9)	0.3739(6)	4.6(2)					
C(2)	0.0835(6)	0.0362(10)	0.4223(6)	5.3(2)					
C(3)	0.0139(5)	0.2640(9)	0.3721(6)	4.8(2)					
C(4)	-0.0393(6)	0.2680(11)	0.4383(7)	6.0(3)					
C(5)	0.1503(5)	0.7080(9)	0.2820(5)	4.2(2)					
C(6)	0.2531(7)	0.3737(10)	0.3486(7)	6.1(3)					
C(7)	0.2366(8)	0.3470(14)	0.4306(8)	8.7(4)					
C(8)	0.1695(6)	0.5278(11)	0.2904(7)	6.5(3)					
C(9)	0.1255(8)	0.5823(14)	0.3535(9)	9.2(4)					
C(10)	0.1344(5)	-0.0125(9)	0.1781(5)	4.2(2)					
C(11)	0.1514(6)	-0.2308(11)	0.1662(7)	6.2(3)					
C(12)	0.0922(8)	-0.2873(13)	0.1199(8)	8.6(4)					
C(13)	0.2067(6)	-0.0846(10)	0.0768(6)	5.7(3)					
C(14)	0.2664(8)	-0.0973(14)	0.0942(8)	8.6(4)					

[a] THE FORM OF THE ANISOTROPIC THERMAL PARAMETER IS: $\exp[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}\ell^2+\beta_{12}hk+\beta_{13}h\ell+\beta_{23}k\ell)]$.

Table II. POSITIONAL AND THERMAL PARAMETERS AND THEIR ESTIMATED STANDARD DEVIATIONS for $Cr_2(O_2CNEt_2)_4(HNEt_2)_2$[a]

Atom	X	Y	Z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Cr	0.0867(1)	-0.0433(1)	0.0052(1)	0.0137(1)	0.0106(1)	0.0171(1)	0.0064(2)	0.0087(2)	0.0097(2)
O(1)	0.0334(5)	-0.1076(4)	0.1927(5)	0.0165(6)	0.0156(5)	0.0198(7)	0.0109(9)	0.011(1)	0.018(1)
O(2)	-0.1278(5)	-0.0258(5)	0.1851(5)	0.0176(6)	0.0153(5)	0.0221(7)	0.0125(9)	0.018(1)	0.016(1)
O(3)	0.2097(5)	0.1296(4)	0.1398(6)	0.0140(6)	0.0121(5)	0.0255(9)	0.0033(10)	0.002(1)	0.009(1)
O(4)	0.0469(5)	0.2113(4)	0.1316(6)	0.0166(6)	0.0116(5)	0.0222(8)	0.0081(9)	0.010(1)	0.006(1)
N(1)	-0.1036(6)	-0.1449(6)	0.3615(7)	0.0179(8)	0.0134(6)	0.0184(9)	0.004(1)	0.012(1)	0.012(1)
N(2)	0.2551(7)	0.3418(6)	0.2396(9)	0.0180(9)	0.0118(7)	0.0335(15)	0.002(1)	0.004(2)	0.005(2)
N(3)	0.2595(9)	-0.1396(9)	0.0153(11)	0.0334(12)	0.0386(12)	0.0315(17)	0.047(2)	-0.003(2)	0.012(2)
C(1)	-0.0636(7)	-0.0919(7)	0.2408(8)	0.0163(9)	0.0119(7)	0.016(1)	0.005(1)	0.008(2)	0.011(1)
C(2)	-0.0325(9)	-0.2170(8)	0.4323(9)	0.0256(13)	0.0170(8)	0.022(1)	0.016(2)	0.007(2)	0.022(2)
C(3)	-0.0799(13)	-0.3579(10)	0.3438(15)	0.0404(20)	0.0186(11)	0.040(2)	0.029(2)	0.012(4)	0.011(3)
C(4)	-0.2117(8)	-0.1242(8)	0.4225(9)	0.0191(10)	0.0194(11)	0.023(1)	0.006(2)	0.021(2)	0.013(2)
C(5)	-0.3442(11)	-0.2238(13)	0.3378(15)	0.0213(15)	0.0333(20)	0.042(3)	0.009(3)	0.013(3)	0.009(4)
C(6)	0.1666(8)	0.2224(7)	0.1650(9)	0.0159(10)	0.0117(8)	0.019(1)	0.002(1)	0.003(2)	0.006(2)
C(7)	0.2098(11)	0.4507(9)	0.2743(14)	0.0283(17)	0.0154(11)	0.045(3)	0.012(2)	0.001(4)	0.013(3)
C(8)	0.2019(18)	0.5073(14)	0.1544(22)	0.0484(30)	0.0311(20)	0.079(5)	0.031(4)	0.042(6)	0.033(5)
C(9)	0.3979(10)	0.3595(10)	0.2834(14)	0.0182(13)	0.0172(12)	0.046(3)	-0.000(2)	0.001(3)	-0.006(3)
C(10)	0.4522(13)	0.3797(13)	0.1373(17)	0.0298(18)	0.0314(20)	0.059(3)	0.014(3)	0.039(4)	0.013(4)
C(11B)[b]	0.378(2)	-0.077(2)	0.123(3)	12.3(7)					
C(11A)[b]	0.317(3)	-0.151(3)	0.135(4)	15.1(10)					
C(12)	0.356(1)	-0.068(1)	0.280(2)	12.8(4)					
C(13A)[b]	0.319(3)	-0.142(2)	-0.125(3)	12.4(8)					
C(13B)[b]	0.215(3)	-0.267(2)	-0.138(3)	12.5(8)					
C(14)	0.240(2)	-0.222(2)	-0.245(2)	16.0(5)					

---

[a] THE FORM OF THE ANISOTROPIC THERMAL PARAMETER IS: $\exp[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}\ell^2+\beta_{12}hk+\beta_{13}h\ell+\beta_{23}k\ell)]$.

[b] Refined at 0.5 occupancy.

Table III. Bond Distances (Å) and Angles (Deg) in $Cr_2(O_2CNEt_2)_4(NEt_2)_2$.[a]

Atoms	Distance	Atoms	Angle
Cr-Cr'	2.948(2)	O(1)-Cr-N(1)'	99.1(2)
-O(1)	1.993(4)	O(2)-Cr-O(3)	98.0(2)
-O(2)	2.066(5)	-O(4)	86.7(2)
-O(3)	1.988(5)	-N(1)	95.5(2)
-O(4)	2.063(4)	-N(1)'	163.9(2)
-N(1)	2.046(5)	O(3)-Cr-O(4)	65.0(2)
-N(1)'	2.045(5)	-N(1)	98.9(2)
N(1)-N(1)'	2.84(1)	-N(1)'	97.1(2)
-C(1)	1.503(8)	O(4)-Cr-N(1)	163.8(2)
-C(3)	1.494(8)	-N(1)'	94.5(2)
C(1)-C(2)	1.55(1)	N(1)-Cr-N(1)'	87.8(2)
C(3)-C(4)	1.57(1)	Cr-N(1)-Cr'	92.2(2)
O(1)-O(2)	2.179(6)	-C(1)	112.0(4)
C(5)-O(1)	1.285(8)	-C(3)	113.3(4)
-O(2)	1.273(8)	Cr'-N(1)-C(1)	113.3(4)
-N(2)	1.347(8)	-C(3)	111.6(4)
N(2)-C(6)	1.47(1)	C(1)-N(1)-C(3)	112.8(5)
-C(8)	1.48(1)	N(1)-C(1)-C(2)	113.4(6)
C(6)-C(7)	1.55(1)	N(1)-C(3)-C(4)	113.6(6)
C(8)-C(9)	1.54(1)	Cr-O(1)-C(5)	90.6(4)
O(3)-O(4)	2.177(6)	Cr-O(2)-C(5)	87.7(4)
C(10)-O(3)	1.277(8)	O(1)-C(5)-O(2)	116.8(7)
-O(4)	1.272(8)	N(2)-C(5)-O(1)	121.2(7)
-N(3)	1.342(8)	-O(2)	122.0(7)
N(3)-C(11)	1.45(1)	C(5)-N(2)-C(6)	118.3(7)
-C(13)	1.47(1)	-C(8)	120.7(7)
C(11)-C(12)	1.54(1)	C(6)-N(2)-C(8)	120.8(7)
C(13)-C(14)	1.56(1)	N(2)-C(6)-C(7)	110.8(8)
Atoms	**Angle**	N(2)-C(8)-C(9)	110.4(8)
Cr'-Cr -O(1)	101.0(1)	Cr-O(3)-C(10)	90.4(4)
-O(2)	137.4(1)	Cr-O(4)-C(10)	87.2(4)

Table III. (continued)

Atoms	Angle	Atoms	Angle
Cr'-Cr-O(3)	100.6(1)	O(3)-C(10)-O(4)	117.3(7)
-O(4)	135.9(2)	N(3)-C(10)-O(3)	121.3(7)
-N(1)	43.9(2)	-O(4)	121.4(7)
-N(1)'	43.9(2)	C(10)-N(3)-C(11)	121.4(7)
O(1)-Cr-O(2)	64.9(2)	-C(13)	119.5(7)
-O(3)	158.4(2)	C(11)-N(3)-C(13)	118.9(6)
-O(4)	99.4(2)	N(3)-C(11)-C(12)	110.6(8)
-N(1)	96.0(2)	N(3)-C(13)-C(14)	110.9(7)

[a]Atoms are labelled as in Figure . Estimated standard deviations in the least significant digits are in parentheses.

Table IV. Bond Distances (Å) and Angles (Deg) in $Cr_2(O_2CNEt_2)_4(HNEt_2)_2$.

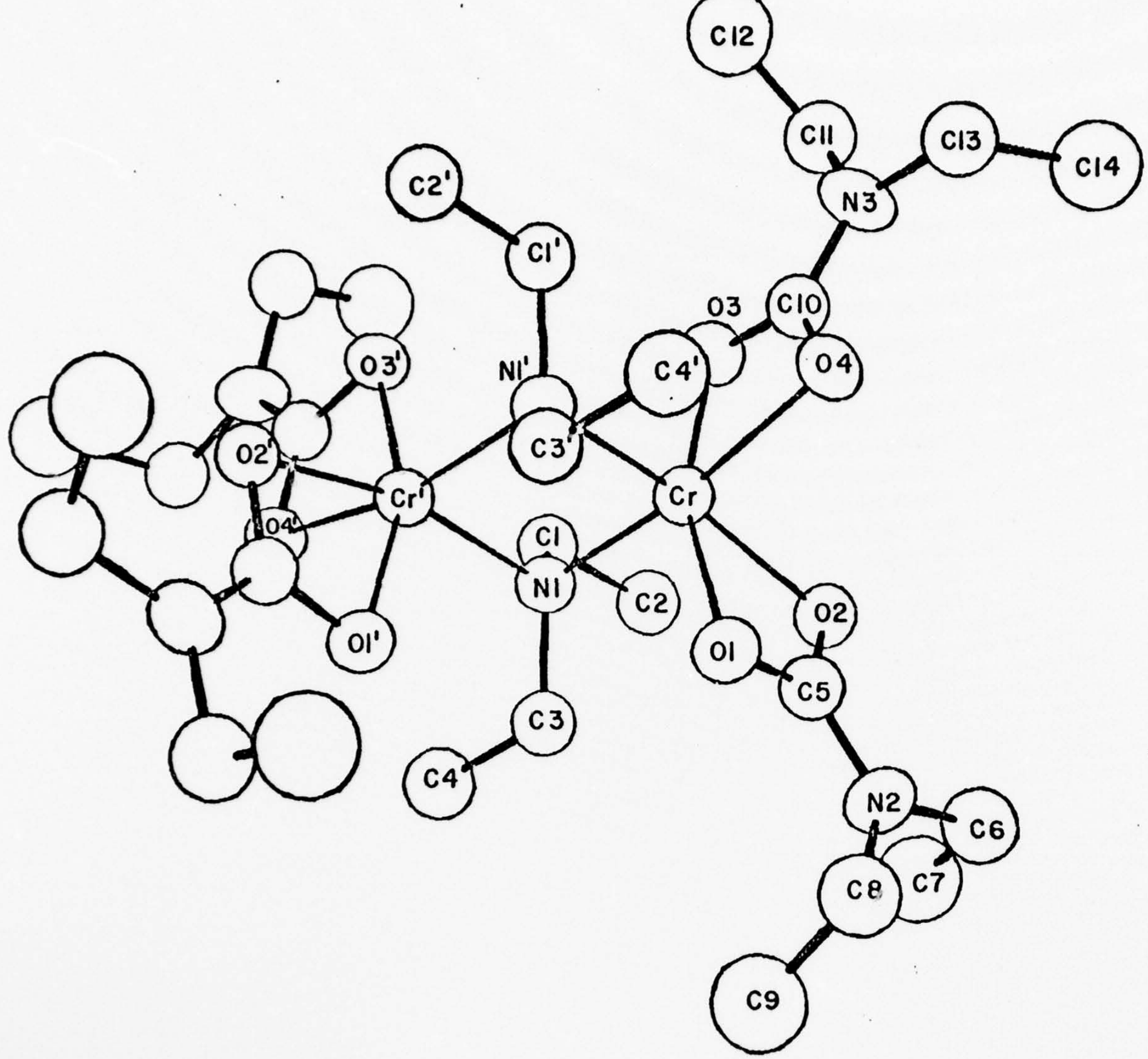
ATOMS	DISTANCE	ATOMS	DISTANCE
Cr-Cr'	2.384(2)	C(6)-O(4)	1.259(7)
-O(1)	2.009(4)	-N(2)	1.361(7)
-O(2)'	2.019(4)	N(2)-C(7)	1.458(10)
-O(3)	2.018(4)	-C(9)	1.492(10)
-O(4)'	2.026(4)	C(7)-C(8)	1.329(15)
-N(3)	2.452(8)	C(9)-C(10)	1.524(13)
C(1)-O(1)	1.252(7)	N(3)-C(11A)	1.20(3)
-O(2)	1.276(7)	-C(11B)	1.38(3)
-N(1)	1.368(7)	-C(13A)	1.49(2)
N(1)-C(2)	1.437(8)	-C(13B)	1.68(2)
-C(4)	1.438(8)	C(11)A-C(12)	1.38(3)
C(2)-C(3)	1.521(10)	C(11)B-C(12)	1.45(3)
C(4)-C(5)	1.509(11)	C(13)A-C(14)	1.27(2)
C(6)-O(3)	1.271(8)	C(13)B-C(14)	1.18(2)

ATOMS	ANGLE	ATOMS	ANGLE
Cr'-Cr-O(1)	87.7(1)	C(2)-N(1)-C(4)	119.9(5)
-O(2)'	87.8(1)	N(1)-C(2)-C(3)	112.2(6)
-O(3)	88.2(1)	N(1)-C(4)-C(5)	113.1(7)
-O(4)'	87.8(1)	Cr-O(3)-C(6)	119.1(4)
-N(3)	178.1(3)	Cr'-O(4)-C(6)	119.2(4)
O(1)-Cr-O(2)'	175.5(2)	O(3)-C(6)-O(4)	124.8(6)
-O(3)	91.9(2)	-N(2)	117.9(7)
-O(4)	88.2(2)	O(4)-C(6)-N(2)	117.2(7)
O(2)'-Cr-O(3)	88.4(2)	C(6)-N(2)-C(7)	119.8(7)
-O(4)'	91.1(2)	-C(9)	119.2(7)
O(3)-Cr-O(4)'	176.0(2)	C(7)-N(2)-C(9)	120.9(6)
N(3)-Cr-O(1)	91.2(3)	N(2)-C(7)-C(8)	112(1)
-O(2)'	93.3(3)	N(2)-C(9)-C(10)	105.7(8)
-O(3)	93.5(3)	Cr-N(3)-C(11A)	123(2)
-O(4)'	90.5(3)	-C(11B)	120(1)

Table IV. (Continued)

ATOMS	ANGLE	ATOMS	ANGLE
Cr-O(1)-C(1)	121.0(4)	Cr-N(3)-C(13A)	114(1)
Cr'-O(2)-C(1)	119.8(4)	-C(13B)	109(1)
O(1)-C(1)-O(2)	123.4(5)	C(11)A-N(3)-C(13A)	120(2)
-N(1)	119.7(6)	C(11)B-N(3)-C(13B)	131(1)
O(2)-C(1)-N(1)	116.8(6)	N(3)-C(11A)-C(12)	128(3)
C(1)-N(1)-C(2)	120.7(6)	N(3)-C(11B)-C(12)	111(2)
-C(4)	120.7(6)	N(3)-C(13A)-C(14)	112(2)
		N(3)-C(13B)-C(14)	105(2)

Fig. 1. A view of the $Cr_2(O_2CNEt_2)_4(\mu\text{-}NEt_2)_2$ molecule with 40% probability ellipsoids of thermal vibration representing the atoms, and showing the atom labelling scheme. The molecule has C_2 symmetry.



C12
C11
C13
C14
C2'
N3
C1'
O3
C10
O3'
N1'
C4'
O4
O2'
C3'
Cr'
Cr
O4'
C1
N1
C2
O2
O1'
O1
C5
C3
C4
N2
C6
C7
C8
C9

Fig. 2. A stereoview of the $Cr_2(O_2CNEt_2)_4(\mu\text{-}NEt_2)_2$ molecule.

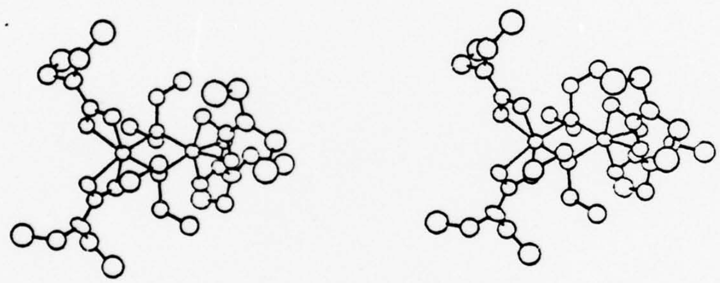
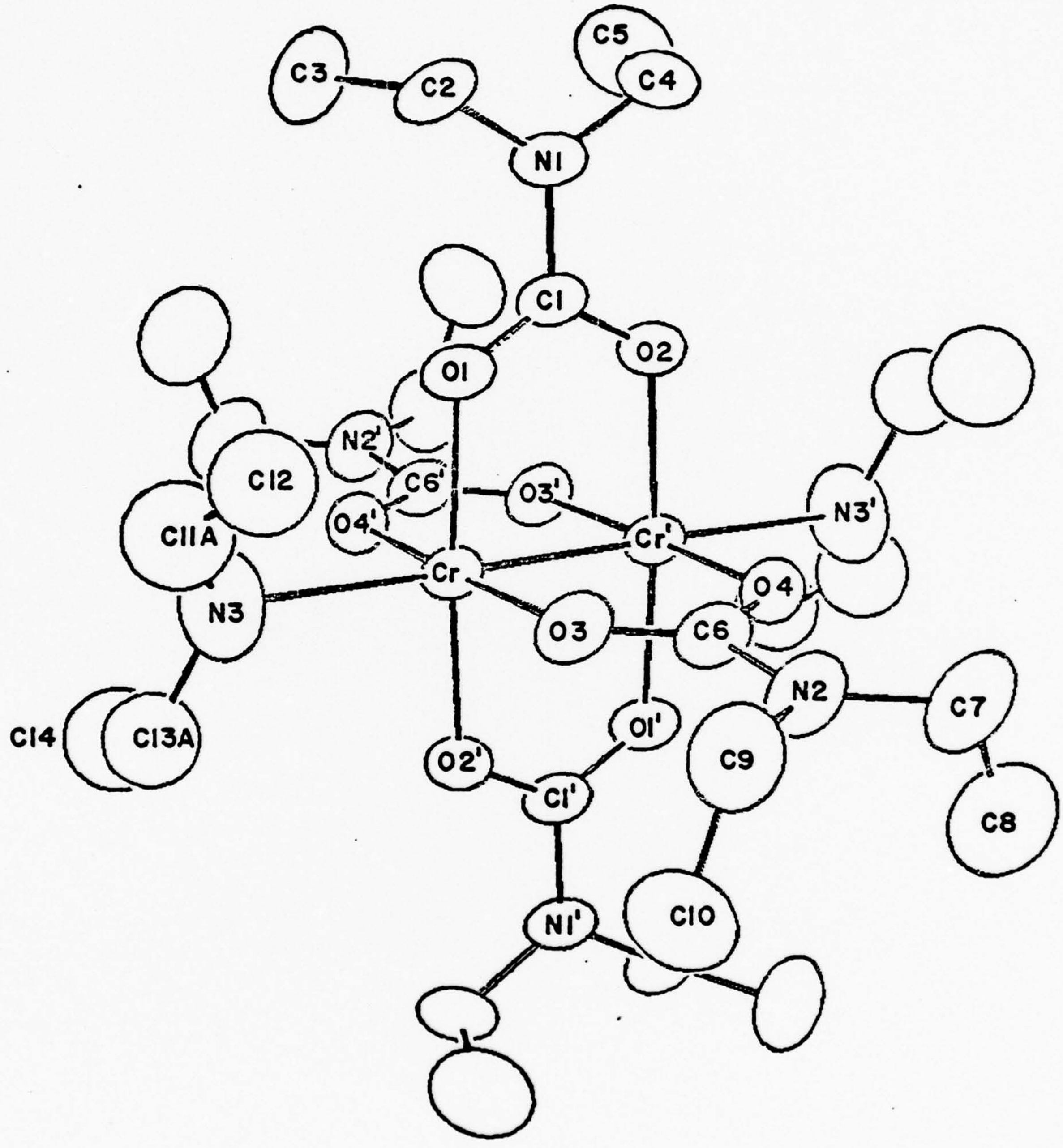


Fig. 3. A view of the $Cr_2(O_2CNEt_2)_4(HNEt_2)_2$ molecule with 30% probability ellipsoids and showing atom labelling scheme. Only one orientation of the disordered methylene groups on N(3) is shown. The molecule has a center of inversion at the midpoint of the Cr-Cr bond.



C3
C2
C5
C4
N1
C1
O1
O2
N2'
C12
C6'
O3'
N3'
O4'
Cr'
C11A
Cr
O4
N3
O3
C6
N2
C7
O1'
C14
C13A
C9
O2'
C1'
C8
N1'
C10

Fig. 1. A view of the $Cr_2(O_2CNEt_2)_4(\mu\text{-}NEt_2)_2$ molecule with 40% probability ellipsoids of thermal vibration representing the atoms, and showing the atom labelling scheme. The molecule has C_2 symmetry.

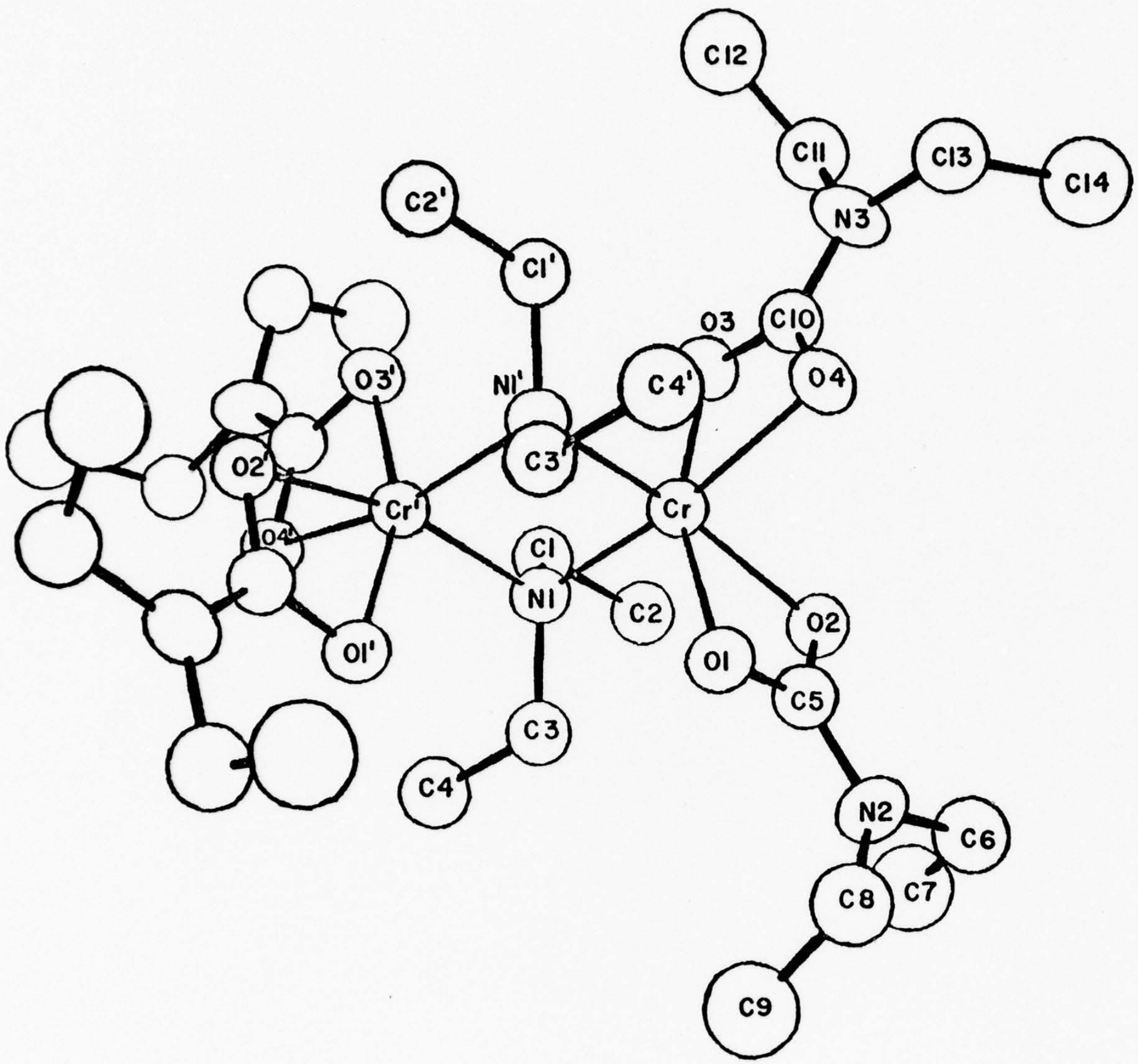

C12
C11
C13
C14
N3
C2'
C1'
C10
O3
O4
N1'
C4'
O3'
C3'
O2'
Cr'
Cr
O4'
C1
N1
C2
O2
O1'
O1
C5
C3
C4
N2
C6
C7
C8
C9

Fig. 2. A stereoview of the $Cr_2(O_2CNEt_2)_4(\mu\text{-}NEt_2)_2$ molecule.

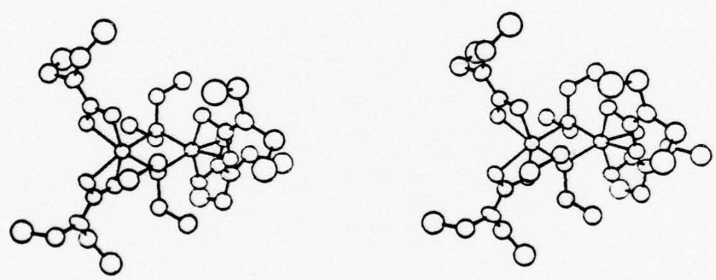
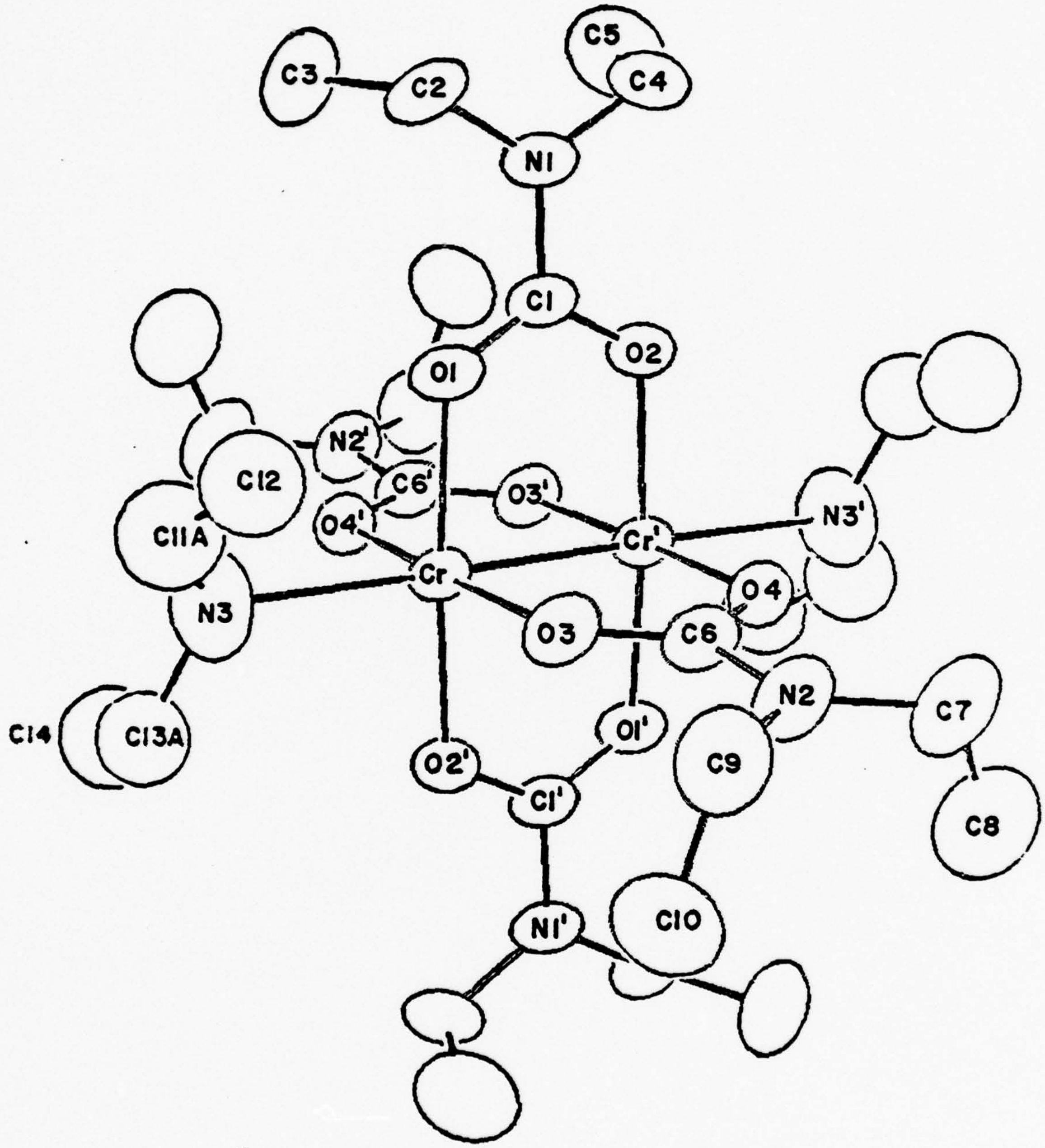


Fig. 3. A view of the $Cr_2(O_2CNEt_2)_4(HNEt_2)_2$ molecule with 30% probability ellipsoids and showing atom labelling scheme. Only one orientation of the disordered methylene groups on N(3) is shown. The molecule has a center of inversion at the midpoint of the Cr-Cr bond.


C3
C2
C5
C4
N1
C1
O1
O2
N2'
C12
C6'
O3'
N3'
O4'
C11A
Cr'
Cr
O4
N3
O3
C6
N2
C7
C14
C13A
O1'
C9
O2'
C1'
C8
N1'
C10

10*FOBS & 10*FCALC FOR CR2(O2CNET2)4(HNET2)2   [COTTON, CHISHOLM ET AL 1978]

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
0	0	2	370	281	0	3	5	89	78	0	9	-7	67	59	1	-8	1	158	145	1	-3	-4	106	105
0	0	3	71	42	0	3	6	87	93	0	9	-6	95	98	1	-8	2	224	237	1	-3	-3	51	5
0	0	4	115	124	0	3	7	48	41	0	9	-4	91	84	1	-8	3	182	187	1	-3	-2	86	80
0	0	5	308	293	0	4	-6	60	68	0	9	-3	190	182	1	-8	4	175	170	1	-3	-1	298	282
0	0	6	179	199	0	4	-5	69	73	0	9	-2	107	115	1	-8	7	117	115	1	-3	0	68	77
0	0	7	138	144	0	4	-4	142	137	0	9	-1	52	61	1	-8	8	79	87	1	-3	1	309	311
0	0	8	79	80	0	4	-3	114	115	0	9	1	63	62	1	-7	-6	43	32	1	-3	2	114	113
0	0	9	44	52	0	4	-2	52	56	0	9	2	98	97	1	-7	-2	158	156	1	-3	3	219	190
0	1	-9	72	63	0	4	-1	79	96	0	9	3	46	47	1	-7	-1	202	210	1	-3	4	119	103
0	1	-8	85	88	0	4	0	127	125	0	10	-6	87	91	1	-7	0	154	145	1	-3	6	90	83
0	1	-7	84	78	0	4	1	323	337	0	10	-5	83	75	1	-7	1	66	64	1	-2	-6	159	149
0	1	-6	81	81	0	4	2	358	340	0	10	-4	52	58	1	-7	2	195	203	1	-2	-5	215	224
0	1	-5	273	250	0	4	6	48	51	0	10	-3	131	129	1	-7	3	144	127	1	-2	-4	34	40
0	1	-4	210	176	0	5	-7	43	33	0	10	-1	44	41	1	-7	4	146	138	1	-2	-2	54	55
0	1	1	475	430	0	5	-6	66	61	0	10	0	71	76	1	-7	5	91	93	1	-2	-1	185	161
0	1	2	267	196	0	5	-5	48	65	0	10	1	63	59	1	-7	6	53	43	1	-2	0	92	61
0	1	3	243	233	0	5	-3	93	98	0	10	2	66	65	1	-7	7	125	126	1	-2	1	104	82
0	1	4	207	193	0	5	-2	52	34	0	11	-2	79	77	1	-7	8	73	73	1	-2	2	441	375
0	1	5	322	341	0	5	-1	34	21	0	11	-1	77	76	1	-6	-4	67	58	1	-2	3	67	78
0	1	6	263	256	0	5	0	68	42	0	11	0	60	67	1	-6	-3	86	90	1	-2	5	48	46
0	1	7	116	118	0	5	1	90	101	1	-11	-1	50	48	1	-6	-2	104	111	1	-1	-8	45	49
0	2	-9	49	41	0	5	2	147	159	1	-11	0	58	60	1	-6	-1	87	88	1	-1	-7	98	94
0	2	-8	59	57	0	5	3	38	21	1	-11	1	53	49	1	-6	0	103	113	1	-1	-6	172	167
0	2	-7	52	43	0	6	-5	56	46	1	-11	2	45	41	1	-6	1	99	79	1	-1	-5	267	262
0	2	-6	45	26	0	6	-4	95	96	1	-11	3	52	56	1	-6	2	95	77	1	-1	-4	84	94
0	2	-5	76	67	0	6	1	48	59	1	-11	5	71	75	1	-6	3	88	98	1	-1	-2	181	202
0	2	-4	404	424	0	6	3	42	33	1	-10	-3	67	67	1	-6	4	187	178	1	-1	1	206	247
0	2	-3	423	401	0	7	-8	53	45	1	-10	-2	91	91	1	-6	5	190	185	1	-1	2	81	53
0	2	-2	367	362	0	7	-7	93	88	1	-10	-1	61	65	1	-6	7	67	74	1	-1	3	106	100
0	2	-1	166	130	0	7	-4	101	105	1	-10	2	97	102	1	-6	8	83	75	1	-1	5	197	184
0	2	0	137	141	0	7	-3	83	89	1	-10	3	195	191	1	-5	-4	87	94	1	-1	6	82	69
0	2	2	80	70	0	7	-2	59	59	1	-10	4	69	71	1	-5	-3	54	55	1	0	-9	71	69
0	2	3	93	100	0	7	-1	42	35	1	-10	6	76	81	1	-5	-2	66	67	1	0	-8	96	95
0	2	4	250	255	0	7	0	120	138	1	-9	-4	64	62	1	-5	-1	192	197	1	0	-7	101	97
0	2	5	278	276	0	7	1	85	74	1	-9	-3	95	91	1	-5	0	163	176	1	0	-6	103	116
0	2	6	170	161	0	7	2	44	53	1	-9	-2	92	92	1	-5	1	200	207	1	0	-5	314	322
0	2	7	44	50	0	7	4	45	30	1	-9	1	169	170	1	-5	2	49	36	1	0	-4	186	181
0	3	-5	128	133	0	7	5	43	24	1	-9	2	195	199	1	-5	3	154	162	1	0	-3	34	27
0	3	-4	465	439	0	8	-8	63	65	1	-9	3	185	182	1	-5	4	69	65	1	0	1	62	99
0	3	-3	328	341	0	8	-7	71	69	1	-9	4	135	138	1	-5	5	157	164	1	0	2	195	234
0	3	-2	148	118	0	8	-6	49	45	1	-9	6	64	72	1	-5	8	75	76	1	0	3	84	130
0	3	-1	184	177	0	8	-4	133	143	1	-9	7	66	66	1	-4	-3	73	71	1	0	4	67	77
0	3	0	114	94	0	8	-3	125	116	1	-8	-5	66	59	1	-4	-1	176	174	1	0	5	263	257
0	3	1	455	428	0	8	-2	148	138	1	-8	-4	76	77	1	-4	1	78	79	1	0	6	188	180
0	3	2	177	230	0	8	-1	117	122	1	-8	-3	50	48	1	-4	3	209	181	1	0	7	58	61
0	3	3	188	189	0	8	3	54	54	1	-8	-1	132	124	1	-4	6	89	81	1	1	-9	74	79
0	3	4	200	177	0	8	4	46	46	1	-8	0	152	146	1	-3	-5	85	81	1	1	-8	87	100

H	K	L	FOBS	FCALC
1	1	-7	96	86
1	1	-6	64	75
1	1	-5	208	200
1	1	-4	557	528
1	1	-3	289	313
1	1	-1	304	283
1	1	0	405	399
1	1	2	52	57
1	1	3	57	47
1	1	4	196	208
1	1	5	305	310
1	1	6	191	182
1	1	7	49	52
1	2	-9	66	65
1	2	-8	86	83
1	2	-6	53	50
1	2	-5	215	208
1	2	-4	893	819
1	2	-3	650	546
1	2	0	448	431
1	2	1	330	391
1	2	2	203	194
1	2	3	344	339
1	2	4	261	253
1	2	5	167	172
1	2	6	148	159
1	2	7	55	54
1	2	8	44	37
1	3	-9	51	40
1	3	-8	56	47
1	3	-6	173	163
1	3	-5	370	356
1	3	-4	459	430
1	3	-3	391	390
1	3	-1	54	42
1	3	0	37	25
1	3	1	704	626
1	3	2	676	682
1	3	3	302	271
1	3	4	99	118
1	3	5	46	42
1	3	6	125	121
1	3	7	61	73
1	3	8	49	37
1	4	-8	52	49
1	4	-7	130	139
1	4	-6	126	120

H	K	L	FOBS	FCALC
1	4	-5	101	104
1	4	-4	165	151
1	4	-3	281	290
1	4	-1	75	65
1	4	0	263	302
1	4	1	535	511
1	4	2	441	430
1	4	4	54	53
1	4	5	46	43
1	4	6	78	73
1	4	7	72	80
1	5	-9	46	53
1	5	-8	50	54
1	5	-7	83	77
1	5	-6	53	48
1	5	-4	77	90
1	5	-3	167	194
1	5	-2	114	97
1	5	-1	152	166
1	5	0	233	244
1	5	1	67	68
1	5	2	211	201
1	5	3	86	78
1	5	5	49	62
1	5	6	53	49
1	5	7	51	49
1	6	-6	46	32
1	6	-3	131	135
1	6	-2	199	191
1	6	-1	68	74
1	6	2	76	73
1	6	3	99	113
1	7	2	50	43
1	7	3	61	58
1	8	-3	61	52
1	8	0	45	51
1	8	2	55	32
1	9	-6	47	60
1	9	-4	43	43
1	9	-3	115	111
1	9	2	46	36
1	10	-5	74	82
1	10	-1	53	49
1	10	0	49	56
1	11	-2	92	87
2	-11	-1	45	40
2	-11	3	74	77

H	K	L	FOBS	FCALC
2	-10	-3	61	74
2	-10	-2	68	70
2	-10	1	78	75
2	-10	2	112	111
2	-10	3	139	143
2	-10	4	61	51
2	-9	-4	76	75
2	-9	-3	69	61
2	-9	-1	43	44
2	-9	0	72	72
2	-9	1	157	164
2	-9	2	152	150
2	-9	3	133	140
2	-9	4	143	146
2	-9	7	71	69
2	-8	-5	65	65
2	-8	-2	111	99
2	-8	-1	222	217
2	-8	0	153	161
2	-8	1	103	107
2	-8	2	256	260
2	-8	3	160	154
2	-8	4	131	129
2	-8	7	107	111
2	-8	8	78	77
2	-7	-6	45	47
2	-7	-3	148	134
2	-7	-2	244	258
2	-7	-1	209	202
2	-7	0	250	245
2	-7	1	136	159
2	-7	2	177	164
2	-7	3	125	136
2	-7	4	190	189
2	-7	5	190	183
2	-7	6	48	31
2	-7	7	93	107
2	-7	8	83	85
2	-6	-4	125	131
2	-6	-3	148	153
2	-6	-2	238	229
2	-6	-1	332	327
2	-6	0	283	281
2	-6	1	42	61
2	-6	2	60	70
2	-6	3	261	253
2	-6	4	238	231

H	K	L	FOBS	FCALC
2	-6	5	272	276
2	-6	6	54	54
2	-6	7	50	57
2	-6	8	106	100
2	-5	-6	76	72
2	-5	-5	52	65
2	-5	-4	75	83
2	-5	-3	211	202
2	-5	-2	207	223
2	-5	-1	159	142
2	-5	0	58	62
2	-5	1	75	78
2	-5	2	95	99
2	-5	3	372	342
2	-5	4	232	230
2	-5	5	238	245
2	-5	6	120	113
2	-5	8	84	90
2	-4	-7	42	27
2	-4	-6	59	64
2	-4	-5	80	83
2	-4	-3	84	76
2	-4	-2	37	45
2	-4	-1	78	65
2	-4	0	228	190
2	-4	1	488	401
2	-4	3	155	139
2	-4	4	207	204
2	-4	5	92	96
2	-4	6	138	150
2	-4	9	53	55
2	-3	-5	43	34
2	-3	-3	61	52
2	-3	-2	213	209
2	-3	-1	328	248
2	-3	0	370	283
2	-3	1	147	103
2	-3	2	86	61
2	-3	3	87	61
2	-3	4	186	166
2	-3	5	104	115
2	-3	6	84	87
2	-3	9	49	45
2	-2	-3	62	51
2	-2	-2	168	141
2	-2	-1	85	52
2	-2	0	508	470

H	K	L	FOBS	FCALC
2	-2	1	295	219
2	-2	2	357	270
2	-2	3	127	129
2	-2	6	38	31
2	-1	-8	49	44
2	-1	-6	48	51
2	-1	-5	120	114
2	-1	-4	41	5
2	-1	-3	169	156
2	-1	-2	73	89
2	-1	-1	209	208
2	-1	0	485	470
2	-1	1	33	51
2	-1	2	206	211
2	-1	3	36	35
2	-1	4	57	44
2	-1	5	45	53
2	0	-9	58	48
2	0	-8	47	63
2	0	-6	54	55
2	0	-5	79	79
2	0	-4	58	78
2	0	-3	187	183
2	0	-2	509	482
2	0	-1	257	221
2	0	0	143	109
2	0	1	291	242
2	0	2	67	53
2	0	3	32	9
2	0	4	43	37
2	0	5	111	110
2	0	6	66	61
2	1	-9	56	56
2	1	-8	70	67
2	1	-7	42	34
2	1	-6	37	35
2	1	-5	130	130
2	1	-4	583	583
2	1	-3	502	486
2	1	-1	257	255
2	1	1	538	552
2	1	3	47	50
2	1	4	167	162
2	1	5	125	116
2	1	6	58	60
2	2	-9	56	54
2	2	-8	62	60

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
2	2	-6	149	157	2	5	-7	96	98	3	-9	2	92	86	3	-5	5	217	206	3	-1	0	457	361
2	2	-5	377	370	2	5	-6	89	94	3	-9	3	64	66	3	-5	6	147	138	3	-1	1	285	242
2	2	-4	603	557	2	5	-5	46	53	3	-9	4	76	77	3	-5	8	53	62	3	-1	2	182	179
2	2	-3	422	429	2	5	-4	61	65	3	-8	-3	59	64	3	-4	-8	45	45	3	-1	3	46	40
2	2	-2	40	40	2	5	-3	277	260	3	-8	-2	115	113	3	-4	-7	79	84	3	-1	5	99	96
2	2	0	154	122	2	5	-2	380	394	3	-8	-1	163	167	3	-4	-6	110	108	3	-1	6	50	44
2	2	1	549	488	2	5	-1	220	223	3	-8	0	148	141	3	-4	-5	171	173	3	-1	7	64	62
2	2	2	450	481	2	5	0	259	236	3	-8	1	43	35	3	-4	-4	76	89	3	0	-8	44	41
2	2	3	204	202	2	5	1	98	106	3	-8	2	120	121	3	-4	-3	88	84	3	0	-6	91	84
2	2	4	118	123	2	5	2	216	224	3	-8	3	59	63	3	-4	-2	90	101	3	0	-4	76	68
2	2	5	49	48	2	5	3	142	145	3	-8	4	83	79	3	-4	-1	330	364	3	0	-3	202	183
2	2	6	81	79	2	5	5	79	74	3	-8	5	69	64	3	-4	0	464	474	3	0	-2	139	126
2	3	-9	55	54	2	5	6	47	53	3	-8	7	47	55	3	-4	1	513	495	3	0	-1	221	216
2	3	-8	68	77	2	6	-8	70	78	3	-7	-4	102	85	3	-4	2	187	194	3	0	2	153	134
2	3	-7	131	139	2	6	-7	52	36	3	-7	-3	152	155	3	-4	3	135	135	3	0	5	43	39
2	3	-6	213	203	2	6	-6	44	39	3	-7	-2	200	211	3	-4	4	348	335	3	1	-5	110	114
2	3	-5	280	302	2	6	-5	41	32	3	-7	-1	221	226	3	-4	5	175	167	3	1	-4	234	248
2	3	-4	273	235	2	6	-4	110	120	3	-7	0	234	251	3	-4	6	142	152	3	1	-2	113	109
2	3	-3	395	374	2	6	-3	258	260	3	-7	3	181	188	3	-3	-7	84	92	3	1	-1	79	84
2	3	-2	100	114	2	6	-2	329	341	3	-7	4	212	194	3	-3	-6	95	100	3	1	0	76	62
2	3	-1	52	64	2	6	-1	115	117	3	-7	5	156	155	3	-3	-5	123	120	3	1	1	294	269
2	3	0	217	248	2	6	0	71	81	3	-7	8	62	59	3	-3	-2	102	100	3	1	2	49	65
2	3	1	690	670	2	6	1	51	44	3	-6	-6	78	67	3	-3	-1	254	272	3	1	3	34	33
2	3	2	554	525	2	6	2	61	62	3	-6	-5	81	70	3	-3	0	464	427	3	1	5	42	29
2	3	3	44	57	2	6	3	157	158	3	-6	-4	125	134	3	-3	1	400	380	3	2	-7	74	87
2	3	4	73	85	2	6	4	49	52	3	-6	-3	206	189	3	-3	2	314	318	3	2	-6	126	124
2	3	5	60	44	2	7	-8	54	46	3	-6	-2	327	324	3	-3	4	215	207	3	2	-5	121	114
2	3	6	83	77	2	7	-6	46	33	3	-6	-1	324	331	3	-3	5	133	138	3	2	-4	158	160
2	3	7	74	72	2	7	-5	82	89	3	-6	0	117	118	3	-3	6	90	92	3	2	-3	192	217
2	4	-9	76	89	2	7	-4	95	111	3	-6	2	74	74	3	-3	7	86	84	3	2	-2	56	60
2	4	-8	103	106	2	7	-3	105	98	3	-6	3	329	314	3	-2	-7	52	51	3	2	-1	53	66
2	4	-7	174	170	2	7	-2	137	137	3	-6	4	241	249	3	-2	-6	49	51	3	2	1	288	326
2	4	-6	97	97	2	7	-1	81	88	3	-6	5	212	230	3	-2	-4	53	46	3	2	2	268	264
2	4	-5	144	152	2	7	1	53	50	3	-6	6	78	69	3	-2	-3	57	54	3	3	-9	68	66
2	4	-4	254	224	2	7	2	61	47	3	-6	8	70	73	3	-2	-2	250	255	3	3	-8	74	80
2	4	-3	310	286	2	7	3	96	92	3	-5	-7	74	53	3	-2	-1	128	148	3	3	-7	147	154
2	4	-2	210	231	2	7	4	54	60	3	-5	-6	137	129	3	-2	0	470	344	3	3	-6	108	96
2	4	-1	324	340	2	8	-5	58	60	3	-5	-5	102	105	3	-2	1	104	126	3	3	-5	76	85
2	4	0	311	288	2	8	-2	44	55	3	-5	-4	138	123	3	-2	2	127	117	3	3	-4	174	179
2	4	1	236	206	2	8	-1	67	78	3	-5	-3	302	302	3	-2	5	97	90	3	3	-3	255	290
2	4	2	420	438	2	8	3	56	55	3	-5	-2	188	200	3	-2	6	94	105	3	3	-2	33	25
2	4	3	107	107	3	-11	3	46	44	3	-5	-1	136	146	3	-2	7	103	102	3	3	-1	110	104
2	4	5	73	81	3	-10	1	62	61	3	-5	0	228	269	3	-1	-5	74	76	3	3	0	231	258
2	4	6	66	66	3	-10	3	43	50	3	-5	1	382	381	3	-1	-4	133	122	3	3	1	202	190
2	4	7	62	66	3	-9	-1	97	99	3	-5	2	115	139	3	-1	-3	41	26	3	3	2	246	226
2	5	-9	107	103	3	-9	0	51	42	3	-5	3	321	331	3	-1	-2	230	163	3	3	5	48	48
2	5	-8	87	96	3	-9	1	43	50	3	-5	4	327	329	3	-1	-1	303	231	3	4	-9	109	114

10*FOBS & 10*FCALC FOR CR2(O2CNET2)4(HNET2)2 [COTTON, CHISHOLM ET AL 1978]

H	K	L	FOBS	FCALC
3	4	-8	103	105
3	4	-7	132	125
3	4	-6	89	96
3	4	-5	81	81
3	4	-4	114	116
3	4	-3	270	264
3	4	-2	313	309
3	4	-1	191	198
3	4	0	224	222
3	4	1	67	76
3	4	2	202	204
3	4	3	112	114
3	4	5	56	58
3	5	-8	100	106
3	5	-7	87	82
3	5	-6	88	92
3	5	-4	140	120
3	5	-3	343	343
3	5	-2	416	436
3	5	-1	137	122
3	5	0	118	138
3	5	1	80	72
3	5	2	89	89
3	5	3	166	180
3	5	4	49	49
3	6	-8	98	99
3	6	-7	52	56
3	6	-6	79	82
3	6	-5	119	113
3	6	-4	189	188
3	6	-3	214	205
3	6	-2	261	279
3	6	-1	135	117
3	6	1	98	111
3	6	2	101	98
3	6	3	139	132
3	6	4	70	70
3	6	5	50	42
3	7	-8	71	72
3	7	-7	75	73
3	7	-6	91	95
3	7	-5	101	109
3	7	-4	105	107
3	7	-3	120	114
3	7	-2	132	139
3	7	-1	144	138
3	7	0	44	49

H	K	L	FOBS	FCALC
3	7	1	84	85
3	7	2	61	60
3	7	3	82	88
3	7	4	92	90
3	8	-7	71	79
3	8	-6	56	62
3	8	-5	78	76
3	8	-4	61	60
3	8	-3	68	64
3	8	-2	79	76
3	8	-1	114	107
3	8	2	56	66
3	8	3	70	67
3	9	-3	49	37
3	9	-1	53	54
3	9	0	68	50
3	9	1	62	51
4	-10	2	45	49
4	-9	-1	68	69
4	-8	-3	70	67
4	-8	-2	61	63
4	-8	-1	71	77
4	-8	0	76	74
4	-8	4	42	53
4	-8	5	56	52
4	-7	-4	48	60
4	-7	-3	68	78
4	-7	-2	118	128
4	-7	-1	102	109
4	-7	0	60	61
4	-7	3	120	123
4	-7	4	105	107
4	-7	5	77	74
4	-6	-6	78	79
4	-6	-5	78	74
4	-6	-4	90	92
4	-6	-3	137	142
4	-6	-2	167	168
4	-6	-1	162	181
4	-6	2	55	60
4	-6	3	164	160
4	-6	4	129	130
4	-6	5	118	130
4	-5	-7	72	66
4	-5	-6	119	118
4	-5	-5	176	169
4	-5	-4	131	135

H	K	L	FOBS	FCALC
4	-5	-3	151	171
4	-5	-2	80	79
4	-5	-1	195	206
4	-5	0	232	226
4	-5	1	185	160
4	-5	2	119	134
4	-5	3	252	228
4	-5	4	213	205
4	-5	5	116	118
4	-5	6	102	104
4	-4	-7	107	110
4	-4	-6	165	147
4	-4	-5	223	237
4	-4	-4	71	65
4	-4	-3	70	67
4	-4	-2	221	227
4	-4	-1	362	336
4	-4	0	385	399
4	-4	1	393	393
4	-4	2	280	275
4	-4	3	117	120
4	-4	4	236	248
4	-4	5	131	129
4	-4	6	117	112
4	-3	-8	45	31
4	-3	-7	140	130
4	-3	-6	114	115
4	-3	-5	152	145
4	-3	-4	117	121
4	-3	-3	75	93
4	-3	-2	243	243
4	-3	-1	417	445
4	-3	0	768	751
4	-3	1	416	420
4	-3	2	259	261
4	-3	3	76	79
4	-3	4	144	141
4	-3	5	165	158
4	-3	6	134	135
4	-3	7	115	124
4	-2	-9	53	54
4	-2	-7	72	63
4	-2	-6	69	78
4	-2	-5	130	138
4	-2	-4	229	234
4	-2	-2	322	345
4	-2	-1	461	463

H	K	L	FOBS	FCALC
4	-2	0	543	519
4	-2	1	344	334
4	-2	2	152	153
4	-2	3	44	50
4	-2	4	73	69
4	-2	5	208	220
4	-2	6	150	153
4	-2	7	120	121
4	-1	-9	53	45
4	-1	-6	119	121
4	-1	-5	96	98
4	-1	-4	220	230
4	-1	-2	75	68
4	-1	-1	413	410
4	-1	0	371	346
4	-1	1	224	250
4	-1	2	44	60
4	-1	3	86	91
4	-1	4	104	106
4	-1	5	163	160
4	-1	6	109	106
4	-1	7	81	85
4	0	-6	117	111
4	0	-5	36	25
4	0	-4	101	92
4	0	-3	226	226
4	0	-1	273	242
4	0	0	84	83
4	0	1	94	93
4	0	2	118	138
4	0	3	206	203
4	0	4	43	34
4	0	5	69	73
4	0	6	83	90
4	1	-8	49	39
4	1	-5	76	67
4	1	-3	150	171
4	1	-2	66	59
4	1	-1	240	238
4	1	0	138	144
4	1	1	188	181
4	1	3	104	98
4	1	4	78	80
4	2	-7	58	47
4	2	-6	67	65
4	2	-5	41	42
4	2	-3	62	48

H	K	L	FOBS	FCALC
4	2	-2	69	48
4	2	0	36	58
4	2	2	64	72
4	2	3	62	65
4	2	4	76	78
4	3	-8	57	51
4	3	-7	54	54
4	3	-3	73	83
4	3	-2	100	84
4	3	-1	74	87
4	3	0	106	101
4	4	-9	89	77
4	4	-8	63	73
4	4	-7	48	40
4	4	-4	56	62
4	4	-3	180	192
4	4	-2	237	244
4	4	-1	80	82
4	4	2	54	42
4	4	3	97	94
4	5	-8	86	89
4	5	-7	49	41
4	5	-6	63	51
4	5	-5	74	73
4	5	-4	142	162
4	5	-3	185	191
4	5	-2	205	212
4	5	-1	76	72
4	5	1	49	43
4	5	2	61	58
4	5	3	97	97
4	6	-8	95	86
4	6	-7	72	67
4	6	-6	95	94
4	6	-5	121	119
4	6	-4	130	131
4	6	-3	121	119
4	6	-2	137	142
4	6	-1	119	123
4	6	1	71	77
4	6	2	54	44
4	6	3	72	78
4	6	4	72	74
4	7	-7	101	106
4	7	-6	92	98
4	7	-5	103	98
4	7	-4	82	81

10*FOBS & 10*FCALC FOR CR2(O2CNET2)4(HNET2)2 [COTTON, CHISHOLM ET AL 1978]

H	K	L	FOBS	FCALC
4	7	-3	93	100
4	7	-2	82	88
4	7	-1	130	132
4	7	0	77	66
4	7	2	61	68
4	7	3	82	82
4	8	-6	73	72
4	8	-5	82	73
4	8	-4	60	49
4	8	-3	59	63
4	8	-2	85	75
4	8	-1	93	91
4	8	0	77	77
4	8	1	76	74
4	8	2	65	69
4	9	-4	51	51
4	9	-2	54	47
4	9	-1	76	76
4	9	0	99	94
5	-11	-2	46	35
5	-11	-1	51	34
5	-11	1	55	54
5	-11	2	93	95
5	-11	3	60	65
5	-11	4	54	55
5	-10	-3	56	43
5	-10	-2	51	44
5	-10	0	44	52
5	-10	1	52	51
5	-10	2	93	97
5	-10	3	60	51
5	-9	0	46	50
5	-9	1	50	42
5	-9	3	56	69
5	-9	6	44	34
5	-8	6	45	46
5	-6	-6	44	48
5	-6	-3	55	67
5	-6	0	80	70
5	-6	1	97	83
5	-6	4	39	21
5	-6	5	53	53
5	-5	-7	51	60
5	-5	-6	84	92
5	-5	-5	119	132
5	-5	-1	105	96
5	-5	0	221	226

H	K	L	FOBS	FCALC
5	-5	1	190	176
5	-5	4	61	71
5	-4	-7	89	97
5	-4	-6	102	99
5	-4	-5	133	140
5	-4	-4	39	37
5	-4	-2	256	247
5	-4	-1	217	226
5	-4	0	152	166
5	-4	1	216	214
5	-4	2	131	122
5	-4	4	80	85
5	-4	5	48	55
5	-4	6	47	55
5	-4	7	49	40
5	-3	-7	96	84
5	-3	-6	118	112
5	-3	-5	154	153
5	-3	-4	201	218
5	-3	-3	58	61
5	-3	-2	235	225
5	-3	-1	308	308
5	-3	0	270	279
5	-3	1	269	259
5	-3	2	267	247
5	-3	5	153	160
5	-3	6	101	97
5	-3	7	71	71
5	-2	-6	145	149
5	-2	-5	170	169
5	-2	-4	321	308
5	-2	-3	179	189
5	-2	-2	226	239
5	-2	-1	345	325
5	-2	0	360	366
5	-2	1	298	301
5	-2	2	127	124
5	-2	3	96	104
5	-2	4	106	108
5	-2	5	195	200
5	-2	6	111	115
5	-2	7	63	72
5	-1	-9	62	59
5	-1	-8	44	44
5	-1	-6	154	151
5	-1	-5	193	198
5	-1	-4	343	347

H	K	L	FOBS	FCALC
5	-1	-3	274	271
5	-1	-2	109	134
5	-1	-1	400	397
5	-1	0	209	231
5	-1	1	112	125
5	-1	2	197	191
5	-1	3	280	283
5	-1	4	129	132
5	-1	5	130	130
5	-1	6	124	122
5	0	-8	83	79
5	0	-6	116	112
5	0	-5	223	243
5	0	-4	212	219
5	0	-3	323	295
5	0	-2	55	65
5	0	-1	47	61
5	0	0	100	97
5	0	1	281	273
5	0	2	289	310
5	0	3	224	218
5	0	4	102	116
5	0	5	71	72
5	0	6	89	74
5	1	-8	76	82
5	1	-5	191	196
5	1	-4	132	130
5	1	-3	141	129
5	1	-1	59	65
5	1	0	251	261
5	1	1	238	243
5	1	2	150	157
5	1	3	137	144
5	1	4	101	107
5	2	-7	43	45
5	2	-5	116	103
5	2	-4	117	129
5	2	-3	36	47
5	2	-2	78	77
5	2	-1	89	91
5	2	0	87	89
5	2	1	109	111
5	2	2	157	168
5	2	3	75	60
5	2	6	53	36
5	3	-7	53	46
5	3	-4	43	69

H	K	L	FOBS	FCALC
5	3	0	129	141
5	3	1	105	114
5	3	5	45	46
5	4	2	41	44
5	4	4	44	43
5	5	-8	45	46
5	5	-5	65	66
5	5	-4	47	42
5	5	-3	47	31
5	5	-2	47	38
5	5	-1	42	27
5	6	-7	65	59
5	6	-6	61	53
5	6	-5	82	81
5	6	-2	63	63
5	6	-1	77	83
5	6	0	42	19
5	7	-6	68	55
5	7	-5	62	63
5	7	-2	68	63
5	7	-1	75	74
5	7	0	44	36
5	7	2	55	50
5	8	-5	56	47
5	8	-4	54	52
5	8	-3	49	47
5	8	-2	54	50
5	8	-1	65	70
5	8	0	85	83
6	-11	-2	45	46
6	-11	1	70	61
6	-11	2	97	97
6	-11	3	68	58
6	-10	-3	48	49
6	-10	-2	79	78
6	-10	-1	77	62
6	-10	0	94	97
6	-10	1	54	60
6	-10	2	70	67
6	-10	3	80	72
6	-9	-3	45	38
6	-9	-2	132	122
6	-9	-1	81	86
6	-9	1	53	53
6	-9	2	44	38
6	-9	3	96	101
6	-9	4	72	64

H	K	L	FOBS	FCALC
6	-9	5	66	63
6	-9	6	66	58
6	-8	-2	90	90
6	-8	-1	75	80
6	-8	1	75	81
6	-8	3	56	57
6	-8	4	82	95
6	-8	5	88	77
6	-7	-1	82	82
6	-7	0	56	37
6	-7	3	53	65
6	-7	4	78	86
6	-6	-1	62	58
6	-6	2	85	82
6	-5	-3	65	48
6	-5	-2	46	60
6	-5	-1	53	68
6	-5	1	45	47
6	-5	2	44	35
6	-4	-4	48	58
6	-4	-3	39	32
6	-4	-1	115	115
6	-4	0	85	72
6	-4	1	93	105
6	-4	3	84	81
6	-3	-6	79	85
6	-3	-5	51	47
6	-3	-4	104	107
6	-3	-3	67	70
6	-3	-2	43	62
6	-3	-1	200	193
6	-3	0	209	215
6	-3	1	65	50
6	-3	5	68	69
6	-2	-6	118	117
6	-2	-5	155	146
6	-2	-4	209	213
6	-2	-3	213	214
6	-2	-2	89	102
6	-2	-1	97	86
6	-2	0	105	110
6	-2	1	103	109
6	-2	2	66	61
6	-2	3	120	115
6	-2	4	65	56
6	-2	5	60	67
6	-2	6	59	54

10*FOBS & 10*FCALC FOR CR2(O2CNET2)4(HNET2)2 [COTTON, CHISHOLM ET AL 1978]

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
6	-1	-8	74	69	6	2	5	79	63	7	-7	-3	59	53	7	1	-5	87	72	8	-10	-2	65	65
6	-1	-6	119	120	6	3	-8	58	48	7	-7	-1	103	123	7	1	-4	102	112	8	-10	3	45	34
6	-1	-5	217	222	6	3	-7	80	76	7	-7	0	81	89	7	1	-3	135	138	8	-9	-3	45	38
6	-1	-4	235	238	6	3	-4	136	137	7	-7	1	68	59	7	1	-2	215	213	8	-9	-2	60	65
6	-1	-3	252	257	6	3	-3	123	126	7	-7	2	115	125	7	1	-1	74	78	8	-9	-1	80	74
6	-1	-2	62	68	6	3	-2	159	171	7	-7	3	111	112	7	1	0	160	160	8	-9	3	60	58
6	-1	0	67	72	6	3	-1	132	128	7	-7	4	99	95	7	1	1	182	183	8	-9	4	65	68
6	-1	1	287	276	6	3	0	108	113	7	-6	-1	64	59	7	1	2	80	85	8	-8	-5	59	58
6	-1	2	248	238	6	3	1	68	59	7	-6	0	172	159	7	1	5	48	32	8	-8	-4	56	55
6	-1	3	133	132	6	3	3	58	56	7	-6	1	118	116	7	2	-8	78	76	8	-8	-3	48	41
6	-1	4	83	82	6	3	4	83	77	7	-6	2	51	76	7	2	-7	111	102	8	-8	-2	50	36
6	-1	5	61	63	6	3	5	46	53	7	-6	4	51	54	7	2	-4	181	183	8	-8	-1	110	107
6	-1	6	54	49	6	4	-4	74	85	7	-6	5	56	52	7	2	-3	169	176	8	-8	0	60	55
6	0	-8	93	94	6	4	-3	93	83	7	-5	-1	62	70	7	2	-2	200	206	8	-8	2	86	77
6	0	-6	73	66	6	4	-2	116	116	7	-5	0	185	179	7	2	-1	130	126	8	-8	3	90	91
6	0	-5	243	242	6	4	-1	89	88	7	-5	4	42	20	7	2	0	118	119	8	-8	4	75	74
6	0	-4	241	233	6	4	0	41	45	7	-5	5	45	43	7	2	1	105	92	8	-7	-5	84	75
6	0	-3	279	275	6	4	2	77	72	7	-4	-2	81	80	7	2	3	49	48	8	-7	-4	50	33
6	0	-1	35	30	6	4	3	66	56	7	-4	-1	38	28	7	2	4	71	75	8	-7	-3	51	46
6	0	0	243	248	6	5	-3	90	87	7	-3	-5	47	44	7	3	-7	68	71	8	-7	-2	43	45
6	0	1	284	295	6	5	2	46	49	7	-3	-1	76	78	7	3	-6	66	64	8	-7	-1	104	101
6	0	2	235	225	7	-11	0	53	43	7	-3	1	82	74	7	3	-4	137	146	8	-7	0	126	138
6	0	3	143	147	7	-11	1	50	35	7	-2	-5	86	90	7	3	-3	162	155	8	-7	1	109	113
6	0	4	111	108	7	-10	-2	79	91	7	-2	-4	63	72	7	3	-2	175	181	8	-7	2	109	106
6	1	-8	78	85	7	-10	-1	79	79	7	-2	-3	60	67	7	3	-1	143	139	8	-7	3	54	54
6	1	-7	84	85	7	-10	0	74	64	7	-2	-1	38	20	7	3	2	84	83	8	-7	4	54	63
6	1	-5	214	211	7	-10	3	69	68	7	-2	2	43	48	7	3	3	84	87	8	-6	-6	45	39
6	1	-4	178	175	7	-10	4	58	46	7	-1	-8	51	54	7	3	4	62	60	8	-6	-5	84	72
6	1	-3	123	133	7	-9	-4	55	41	7	-1	-5	119	123	7	4	-7	50	52	8	-6	-4	58	55
6	1	-2	134	132	7	-9	-3	54	51	7	-1	-4	156	152	7	4	-6	89	86	8	-6	-3	45	42
6	1	-1	119	131	7	-9	-2	119	126	7	-1	-3	143	156	7	4	-4	82	82	8	-6	-2	51	50
6	1	0	207	210	7	-9	-1	115	102	7	-1	0	99	100	7	4	-3	176	174	8	-6	-1	122	124
6	1	1	197	192	7	-9	0	44	32	7	-1	1	89	99	7	4	-2	95	91	8	-6	0	192	217
6	1	2	246	248	7	-9	1	47	48	7	-1	2	75	88	7	4	-1	49	37	8	-6	1	103	107
6	1	3	136	132	7	-9	3	96	90	7	-1	3	59	60	7	4	1	72	74	8	-6	2	62	56
6	1	6	46	46	7	-9	4	91	90	7	0	-8	78	71	7	4	2	86	88	8	-6	3	49	39
6	2	-8	65	65	7	-9	5	73	73	7	0	-7	60	63	7	4	3	58	55	8	-6	4	69	68
6	2	-7	110	111	7	-8	-4	83	70	7	0	-5	156	157	7	5	-6	65	69	8	-6	5	79	72
6	2	-5	63	65	7	-8	-3	60	68	7	0	-4	141	141	7	5	-5	52	51	8	-5	-5	49	61
6	2	-4	128	110	7	-8	-2	85	74	7	0	-3	102	115	7	5	-4	48	38	8	-5	-4	58	58
6	2	-3	141	133	7	-8	-1	130	131	7	0	-1	38	36	7	5	-3	86	84	8	-5	-2	88	94
6	2	-2	199	219	7	-8	2	56	59	7	0	0	196	196	7	5	0	69	65	8	-5	-1	122	125
6	2	-1	76	77	7	-8	3	121	117	7	0	1	132	137	7	5	2	54	53	8	-5	0	157	156
6	2	0	181	172	7	-8	4	133	138	7	0	2	114	120	7	6	-5	60	48	8	-5	1	67	62
6	2	1	209	222	7	-8	5	66	70	7	0	3	87	81	7	6	-2	46	50	8	-5	3	62	57
6	2	2	117	121	7	-7	-6	51	49	7	1	-8	74	81	7	6	-1	48	40	8	-5	4	45	40
6	2	2	118	121	7	-7	-5	57	56	7	1	-7	110	108	7	6	0	45	35	8	-5	5	88	81

10*FOBS & 10*FCALC FOR CR2(O2CNET2)4(HNET2)2 [COTTON, CHISHOLM ET AL 1978]

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
8	-4	-4	70	68	8	4	1	58	54	9	-2	-6	45	40	10	0	1	44	24					
8	-4	-3	68	75	8	5	-5	79	73	9	-2	-3	61	66	11	-3	-3	50	47					
8	-4	-2	78	86	8	5	-2	63	63	9	-2	-1	51	49	11	-3	0	58	49					
8	-4	0	84	78	8	5	-1	78	69	9	-2	0	44	38	11	-3	1	45	52					
8	-4	1	77	95	8	5	0	64	62	9	-2	1	59	71	11	-2	-3	66	58					
8	-4	3	43	48	9	-8	-1	46	48	9	-2	2	86	84	11	-2	-2	75	68					
8	-4	4	57	49	9	-8	0	72	56	9	-1	-1	42	48	11	-2	-1	62	46					
8	-4	5	55	54	9	-8	1	45	40	9	2	-3	82	91	11	-1	-4	54	48					
8	-3	-4	60	74	9	-7	-5	49	53	9	2	2	43	28	11	-1	-3	64	66					
8	-3	-1	45	28	9	-7	-1	82	78	9	3	-3	78	75	11	-1	-2	78	76					
8	-3	0	49	27	9	-7	0	137	133	9	4	-2	46	40	11	-1	-1	48	40					
8	-3	1	59	60	9	-7	1	74	71	9	4	-1	55	46	11	0	-3	54	48					
8	-3	3	44	40	9	-6	-5	59	59	10	-7	0	71	67	11	0	-2	63	55					
8	-3	4	46	37	9	-6	-2	89	73	10	-6	-4	44	36	11	0	-1	54	36					
8	-2	1	52	49	9	-6	-1	116	114	10	-6	-2	45	49										
8	-1	-5	61	74	9	-6	0	141	143	10	-6	0	60	56										
8	-1	-4	49	45	9	-6	1	66	63	10	-5	-5	53	48										
8	0	-4	49	35	9	-5	-5	51	51	10	-5	-4	87	88										
8	0	-2	69	76	9	-5	-4	83	82	10	-5	-3	73	72										
8	0	0	50	44	9	-5	-3	108	93	10	-5	-2	46	41										
8	0	1	73	86	9	-5	-2	113	112	10	-5	1	78	66										
8	1	-7	74	70	9	-5	-1	62	63	10	-4	-5	76	69										
8	1	-4	104	112	9	-5	0	90	102	10	-4	-4	97	95										
8	1	-3	85	80	9	-5	1	116	100	10	-4	-3	75	63										
8	1	-2	110	103	9	-5	2	51	36	10	-4	-1	53	34										
8	1	-1	65	66	9	-5	3	50	48	10	-4	1	106	99										
8	1	0	44	50	9	-5	5	76	70	10	-4	2	80	74										
8	1	1	58	59	9	-4	-5	74	73	10	-3	-6	59	47										
8	2	-7	63	61	9	-4	-4	129	133	10	-3	-5	59	53										
8	2	-4	116	121	9	-4	-3	92	89	10	-3	-4	81	71										
8	2	-3	117	119	9	-4	-2	46	53	10	-3	-3	78	84										
8	2	-2	131	122	9	-4	0	53	65	10	-3	0	66	59										
8	2	-1	120	118	9	-4	1	129	123	10	-3	1	104	102										
8	2	3	57	50	9	-4	2	70	58	10	-3	2	92	93										
8	3	-7	46	50	9	-4	3	73	72	10	-2	-4	50	43										
8	3	-6	72	72	9	-4	4	70	64	10	-2	-3	68	74										
8	3	-4	88	93	9	-4	5	46	44	10	-2	-2	46	42										
8	3	-3	179	176	9	-3	-6	47	48	10	-2	-1	55	55										
8	3	-2	117	104	9	-3	-5	71	69	10	-2	0	80	79										
8	3	1	49	39	9	-3	-4	80	85	10	-2	1	67	61										
8	3	2	72	73	9	-3	-3	48	45	10	-2	2	73	73										
8	3	3	52	58	9	-3	-2	47	37	10	-1	-3	64	64										
8	4	-6	84	84	9	-3	-1	51	62	10	-1	-2	87	87										
8	4	-5	65	64	9	-3	1	108	114	10	-1	-1	55	44										
8	4	-4	64	61	9	-3	2	105	107	10	-1	0	42	45										
8	4	-3	103	112	9	-3	3	59	45	10	-1	2	47	49										
8	4	0	53	56	9	-3	4	46	40	10	0	-2	61	61										

10*FOBS & 10*FCALC FOR CR2[O2CNET2]4[NET2]2 (CHISHOLM, COTTON ET AL 1977) PAGE 1

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
0	0	4	706	283	0	6	10	298	275	1	1	10	639	632	1	5	4	120	108	1	10	4	153	171
0	0	6	1258	1113	0	6	11	580	535	1	1	11	518	543	1	5	5	888	960	1	10	6	236	262
0	0	8	535	674	0	6	12	343	336	1	1	12	531	525	1	5	6	159	136	1	10	8	210	219
0	0	10	1309	1238	0	6	13	405	410	1	1	13	267	276	1	5	7	435	560	1	10	10	173	152
0	0	12	837	799	0	6	14	367	381	1	1	14	202	197	1	5	8	280	293	1	11	0	303	263
0	0	16	279	295	0	6	15	156	187	1	1	15	312	293	1	5	9	594	563	1	11	1	371	335
0	0	18	186	166	0	6	16	176	171	1	1	16	144	130	1	5	10	255	267	1	11	2	321	289
0	2	0	366	379	0	8	0	285	284	1	1	17	180	170	1	5	11	628	574	1	11	3	271	279
0	2	1	645	755	0	8	1	666	665	1	2	1	228	200	1	5	13	572	580	1	11	4	287	268
0	2	2	284	364	0	8	3	268	193	1	2	3	226	236	1	5	14	139	112	1	11	5	243	205
0	2	3	1559	1544	0	8	5	379	368	1	2	4	102	155	1	5	15	199	223	1	11	6	218	227
0	2	4	530	540	0	8	7	335	328	1	2	5	620	600	1	6	1	270	290	1	11	7	226	198
0	2	5	157	191	0	8	10	237	268	1	2	6	254	257	1	6	2	388	440	1	11	8	150	167
0	2	6	247	287	0	8	11	193	189	1	2	8	142	118	1	6	3	536	496	1	11	9	216	220
0	2	7	456	407	0	8	13	137	111	1	2	9	123	77	1	6	4	132	282	2	0	0	316	387
0	2	8	225	246	0	8	14	154	109	1	2	11	250	205	1	6	5	541	523	2	0	2	820	770
0	2	9	752	747	0	8	15	115	124	1	2	13	185	157	1	6	6	209	190	2	0	4	917	868
0	2	10	207	191	0	10	0	258	222	1	2	15	188	212	1	6	7	331	349	2	0	6	919	982
0	2	11	313	384	0	10	2	279	244	1	2	17	158	171	1	6	8	156	142	2	0	8	1461	1338
0	2	13	461	456	0	10	4	440	408	1	3	0	145	249	1	6	10	240	240	2	0	10	781	768
0	2	15	332	301	0	10	5	221	225	1	3	1	152	198	1	6	16	221	215	2	0	12	263	257
0	4	0	942	1221	0	10	6	485	481	1	3	2	924	984	1	7	0	1009	1014	2	0	14	495	470
0	4	1	443	557	0	10	7	172	157	1	3	3	133	163	1	7	1	247	292	2	0	16	348	362
0	4	2	874	1013	0	10	8	389	367	1	3	4	839	756	1	7	2	727	727	2	0	20	120	138
0	4	3	804	828	0	10	10	313	293	1	3	5	185	180	1	7	3	147	157	2	1	1	670	568
0	4	4	512	462	0	12	1	385	363	1	3	6	190	164	1	7	4	444	489	2	1	2	1571	1476
0	4	5	408	456	0	12	3	351	382	1	3	8	175	177	1	7	5	140	176	2	1	3	999	877
0	4	6	223	295	1	0	2	407	436	1	3	10	326	360	1	7	6	459	472	2	1	4	2068	1840
0	4	7	149	214	1	0	4	598	489	1	3	11	192	202	1	7	7	267	243	2	1	5	216	186
0	4	8	513	541	1	0	6	948	848	1	3	12	369	385	1	7	8	437	426	2	1	6	575	531
0	4	10	777	758	1	0	8	264	243	1	3	13	328	360	1	7	10	371	380	2	1	8	144	120
0	4	12	639	661	1	0	10	183	163	1	3	14	276	250	1	7	11	165	99	2	1	9	155	169
0	4	13	309	319	1	0	12	494	503	1	4	1	557	539	1	7	12	307	273	2	1	10	306	341
0	4	14	144	178	1	0	14	687	675	1	4	4	172	179	1	7	14	217	243	2	1	11	429	401
0	4	15	211	238	1	0	16	468	473	1	4	5	531	548	1	7	16	140	165	2	1	12	499	538
0	4	18	172	148	1	0	18	240	275	1	4	7	279	301	1	8	2	218	153	2	1	13	528	540
0	4	19	139	102	1	0	18	269	274	1	4	8	344	354	1	8	4	231	223	2	1	14	379	393
0	6	0	597	624	1	0	20	218	187	1	4	9	305	292	1	8	6	150	147	2	1	15	442	461
0	6	1	464	474	1	1	0	2123	2410	1	4	10	329	333	1	8	13	127	112	2	1	16	237	237
0	6	2	1301	1305	1	1	2	1006	1154	1	4	11	207	251	1	9	0	207	242	2	1	17	308	311
0	6	3	1061	1084	1	1	3	1323	1461	1	4	12	240	271	1	9	1	226	256	2	1	18	156	147
0	6	4	1621	1598	1	1	4	237	219	1	4	13	294	303	1	9	5	190	199	2	1	19	212	193
0	6	5	717	775	1	1	5	1741	1477	1	4	14	200	187	1	9	6	265	237	2	1	20	174	151
0	6	6	904	947	1	1	6	496	439	1	4	19	134	108	1	9	7	330	309	2	2	0	859	830
0	6	7	396	394	1	1	7	715	677	1	5	0	184	195	1	9	9	275	252	2	2	1	2067	2175
0	6	8	477	505	1	1	8	467	477	1	5	1	1653	1539	1	9	11	182	201	2	2	3	562	349
0	6	9	526	543	1	1	9	511	493	1	5	3	1880	1861	1	9	13	117	110	2	2	5	229	177

10*FOBS & 10*FCALC FOR CR2[O2CNET2]4[NET2]2 (CHISHOLM, COTTON ET AL 1977)

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
2	2	6	184	165	2	6	1	819	823	3	0	6	1177	977	3	4	2	192	191	3	8	11	163	187
2	2	7	242	306	2	6	2	724	687	3	0	8	392	388	3	4	3	337	369	3	8	13	124	87
2	2	8	119	76	2	6	3	486	458	3	0	10	796	822	3	4	4	277	287	3	8	15	149	134
2	2	9	146	172	2	6	4	335	333	3	0	12	922	850	3	4	5	228	240	3	9	0	477	460
2	2	10	216	201	2	6	5	268	277	3	0	14	597	603	3	4	6	134	190	3	9	1	597	584
2	2	11	508	530	2	6	6	181	222	3	0	16	609	636	3	4	8	206	203	3	9	3	263	228
2	2	13	283	289	2	6	8	237	220	3	0	18	414	411	3	4	9	436	457	3	9	4	211	168
2	3	1	264	195	2	6	10	267	240	3	0	20	279	297	3	4	10	385	349	3	9	6	165	142
2	3	3	1014	894	2	6	11	210	210	3	1	0	684	433	3	4	11	359	322	3	9	10	144	181
2	3	4	368	374	2	6	12	403	391	3	1	1	514	282	3	4	12	404	417	3	10	6	186	186
2	3	5	361	352	2	6	14	203	206	3	1	2	520	429	3	4	14	254	282	3	10	8	223	229
2	3	6	237	200	2	7	6	358	335	3	1	3	1272	1124	3	4	15	175	164	3	10	10	191	207
2	3	7	343	343	2	7	8	397	389	3	1	4	309	335	3	4	16	146	143	4	0	0	1499	1861
2	3	9	132	110	2	7	10	267	274	3	1	5	687	684	3	4	17	208	177	4	0	2	2737	2643
2	3	10	238	205	2	7	12	158	139	3	1	6	413	344	3	4	18	166	160	4	0	4	1676	1472
2	3	11	140	149	2	7	16	208	203	3	1	8	160	94	3	5	1	403	382	4	0	6	256	176
2	3	12	434	438	2	8	0	152	139	3	1	9	612	578	3	5	2	128	124	4	0	8	587	557
2	3	14	312	323	2	8	1	342	361	3	1	10	391	361	3	5	3	208	291	4	0	10	419	417
2	3	15	247	194	2	8	2	144	97	3	1	11	458	463	3	5	4	168	184	4	0	12	295	285
2	3	18	121	126	2	8	3	160	133	3	1	12	256	236	3	5	6	128	93	4	1	1	497	473
2	4	0	692	691	2	8	5	148	148	3	1	15	165	141	3	5	7	189	145	4	1	2	1339	1233
2	4	2	968	967	2	8	7	174	149	3	1	19	133	108	3	5	8	413	420	4	1	3	484	591
2	4	3	799	781	2	8	11	198	194	3	2	1	298	261	3	5	10	335	377	4	1	5	1264	1113
2	4	4	1188	1237	2	8	13	127	94	3	2	2	1030	809	3	5	11	187	144	4	1	7	1221	1071
2	4	5	279	245	2	8	15	125	130	3	2	3	178	168	3	5	13	244	234	4	1	8	478	438
2	4	8	169	198	2	9	2	213	210	3	2	4	1027	895	3	5	14	183	213	4	1	9	297	304
2	4	9	300	309	2	9	4	187	167	3	2	6	123	168	3	5	16	157	180	4	1	10	610	590
2	4	10	129	110	2	9	5	222	222	3	2	7	347	384	3	6	2	178	229	4	1	11	458	446
2	4	11	268	264	2	9	7	340	314	3	2	8	194	211	3	6	5	233	186	4	1	12	187	219
2	4	12	287	295	2	9	8	195	218	3	2	9	668	640	3	6	6	277	276	4	1	13	439	403
2	4	13	231	229	2	9	9	275	265	3	2	11	290	333	3	6	7	449	477	4	1	14	337	316
2	4	14	323	342	2	9	10	172	146	3	2	12	185	195	3	6	8	460	455	4	1	15	183	183
2	5	1	192	210	2	9	11	153	139	3	2	13	321	321	3	6	9	269	278	4	1	16	386	372
2	5	2	786	771	2	10	0	612	601	3	2	15	391	378	3	6	10	345	348	4	1	17	215	214
2	5	3	293	296	2	10	2	394	365	3	2	17	201	249	3	6	11	246	248	4	1	19	198	203
2	5	4	173	186	2	10	4	170	117	3	2	19	193	190	3	6	12	318	348	4	2	0	380	375
2	5	5	237	239	2	10	5	142	88	3	3	0	109	100	3	6	13	351	343	4	2	1	825	632
2	5	6	302	231	2	10	6	137	115	3	3	1	143	176	3	6	14	322	334	4	2	2	253	198
2	5	7	420	452	2	10	8	131	116	3	3	2	258	347	3	6	15	253	258	4	2	3	985	721
2	5	8	241	238	2	11	3	171	166	3	3	3	406	412	3	6	16	258	260	4	2	4	272	281
2	5	9	439	438	2	11	5	145	146	3	3	4	517	511	3	6	17	214	222	4	2	6	285	262
2	5	11	349	339	2	11	6	139	99	3	3	5	250	238	3	7	0	450	483	4	2	8	277	284
2	5	13	424	427	2	11	8	159	152	3	3	6	201	196	3	7	2	231	155	4	2	10	181	194
2	5	15	390	397	2	12	1	177	164	3	3	7	323	252	3	8	1	162	214	4	2	11	305	275
2	5	16	189	177	2	12	3	213	219	3	3	10	125	145	3	8	2	238	211	4	2	15	175	125
2	5	17	344	348	3	0	2	806	819	3	3	12	378	412	3	8	5	226	266	4	3	1	146	150
2	6	0	792	793	3	0	4	1451	1331	3	3	14	288	283	3	8	9	158	159	4	3	4	227	215

10*FOBS & 10*FCALC FOR CR2[O2CNET2]4[NET2]2 (CHISHOLM, COTTON ET AL 1977)

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
4	3	5	140	86	4	7	1	177	193	5	1	14	157	151	5	5	11	228	241	6	0	2	299	349
4	3	6	447	426	4	7	2	192	194	5	1	19	153	120	5	5	15	275	247	6	0	4	1921	1997
4	3	7	220	199	4	7	6	175	179	5	2	1	316	249	5	5	17	128	143	6	0	6	2900	2702
4	3	8	498	540	4	7	8	229	234	5	2	2	502	436	5	6	2	156	144	6	0	8	1433	1424
4	3	9	178	151	4	7	9	144	136	5	2	3	477	400	5	6	3	181	145	6	0	10	970	985
4	3	10	273	295	4	7	10	238	258	5	2	4	114	111	5	6	4	433	472	6	0	12	899	842
4	3	12	156	179	4	7	12	378	358	5	2	5	185	216	5	6	5	253	229	6	0	14	377	399
4	3	14	169	182	4	7	14	294	290	5	2	6	446	376	5	6	9	218	184	6	0	16	204	222
4	3	16	171	142	4	7	15	146	127	5	2	9	313	313	5	6	10	391	380	6	0	18	170	146
4	3	18	194	181	4	7	16	224	225	5	2	11	441	457	5	6	11	317	360	6	1	2	758	715
4	3	19	160	150	4	8	0	169	182	5	2	12	187	116	5	6	12	276	295	6	1	3	355	268
4	4	0	244	246	4	8	1	262	300	5	2	13	270	252	5	6	13	260	284	6	1	4	615	483
4	4	1	132	136	4	8	3	175	139	5	2	15	139	100	5	6	14	226	227	6	1	6	509	431
4	4	5	215	211	4	8	5	290	315	5	2	19	196	181	5	6	16	130	92	6	1	7	414	352
4	4	6	264	283	4	8	12	139	91	5	3	0	431	404	5	6	17	117	97	6	1	8	496	413
4	4	7	270	272	4	9	2	195	152	5	3	2	239	232	5	7	0	556	578	6	1	9	157	178
4	4	8	738	719	4	9	3	155	108	5	3	3	323	354	5	7	1	173	172	6	1	15	154	81
4	4	10	366	353	4	9	4	186	159	5	3	4	184	213	5	7	2	480	475	6	2	1	469	431
4	4	11	217	225	4	9	11	176	130	5	3	5	274	244	5	7	3	182	141	6	2	2	168	131
4	4	12	178	163	4	9	12	127	115	5	3	6	423	451	5	7	4	443	485	6	2	3	834	770
4	4	15	160	177	4	9	13	136	148	5	3	7	310	302	5	7	5	221	274	6	2	5	902	911
4	4	17	149	140	4	10	0	176	215	5	3	8	477	493	5	7	6	507	532	6	2	6	178	164
4	5	1	195	184	4	10	4	277	271	5	3	9	180	182	5	7	7	142	152	6	2	7	793	927
4	5	2	318	239	4	10	6	261	297	5	3	10	273	248	5	7	8	358	348	6	2	8	437	453
4	5	3	333	363	4	10	8	150	121	5	3	11	184	176	5	7	10	213	224	6	2	9	602	555
4	5	4	400	448	4	11	4	131	143	5	3	16	165	127	5	7	12	181	153	6	2	10	256	246
4	5	5	254	288	4	11	7	160	121	5	3	18	135	93	5	8	2	297	292	6	2	11	233	215
4	5	7	479	492	4	12	1	119	127	5	4	1	281	334	5	8	4	313	310	6	2	13	141	150
4	5	8	152	167	5	0	2	894	904	5	4	2	247	289	5	8	5	189	170	6	2	14	142	153
4	5	9	723	709	5	0	6	1573	1563	5	4	3	317	316	5	8	7	262	247	6	2	15	154	168
4	5	11	567	560	5	0	8	1754	1625	5	4	5	115	53	5	8	13	158	183	6	2	17	163	192
4	5	13	375	414	5	0	10	789	801	5	4	6	152	144	5	9	1	178	143	6	2	19	115	108
4	5	15	306	300	5	0	16	163	166	5	4	7	132	164	5	9	3	289	268	6	3	1	571	622
4	5	17	243	253	5	0	18	146	150	5	4	8	388	389	5	9	5	249	256	6	3	2	135	188
4	6	0	285	368	5	1	0	896	983	5	4	10	205	185	5	9	6	192	154	6	3	3	428	489
4	6	1	382	453	5	1	1	115	160	5	4	14	187	160	5	10	1	138	50	6	3	4	185	174
4	6	2	414	410	5	1	2	889	962	5	4	16	262	265	5	10	3	184	182	6	3	5	192	119
4	6	3	369	364	5	1	3	1524	1417	5	4	18	241	253	5	10	5	172	101	6	3	6	123	139
4	6	4	711	688	5	1	4	1335	1194	5	5	0	200	126	5	11	0	226	222	6	3	8	190	208
4	6	5	228	185	5	1	5	1526	1425	5	5	1	1060	1092	5	11	1	275	259	6	3	9	426	412
4	6	6	733	733	5	1	6	996	862	5	5	2	199	255	5	11	2	197	165	6	3	10	199	181
4	6	7	244	240	5	1	7	948	890	5	5	3	892	973	5	11	3	282	272	6	3	16	138	132
4	6	8	297	262	5	1	8	127	90	5	5	4	138	97	5	11	4	239	217	6	3	18	198	171
4	6	9	307	299	5	1	9	706	710	5	5	5	772	719	5	11	5	246	246	6	4	0	758	852
4	6	11	179	209	5	1	11	659	655	5	5	7	1008	995	5	11	6	273	267	6	4	1	437	438
4	6	14	170	96	5	1	12	179	248	5	5	9	866	880	5	11	7	226	201	6	4	2	760	780
4	6	16	152	142	5	1	13	354	325	5	5	10	155	187	6	0	0	316	237	6	4	3	402	451

10*FOBS & 10*FCALC FOR CR2[O2CNET2]4[NET2]2 (CHISHOLM, COTTON ET AL 1977)

H	K	L	FOBS	FCALC
6	4	4	797	767
6	4	5	294	275
6	4	6	736	724
6	4	7	671	650
6	4	8	555	560
6	4	9	600	616
6	4	10	312	309
6	4	12	137	123
6	4	14	177	168
6	4	16	180	172
6	4	17	120	66
6	5	5	160	138
6	5	6	367	406
6	5	8	196	163
6	5	9	201	222
6	5	11	173	166
6	6	0	973	1072
6	6	1	647	641
6	6	2	693	731
6	6	3	844	924
6	6	4	485	503
6	6	5	640	623
6	6	6	610	602
6	6	7	452	470
6	6	8	679	630
6	6	9	285	315
6	6	10	571	594
6	6	12	315	338
6	6	14	159	141
6	6	15	136	133
6	6	16	149	148
6	7	3	231	238
6	7	5	167	222
6	7	12	166	167
6	8	2	187	220
6	8	3	342	351
6	8	4	258	268
6	8	5	430	456
6	8	7	291	269
6	8	9	147	145
6	8	11	207	228
6	8	13	199	183
6	10	0	569	562
6	10	2	493	477
6	10	4	420	389
6	10	6	313	288
6	10	8	174	170

H	K	L	FOBS	FCALC
6	10	10	216	180
7	0	4	1421	1313
7	0	6	676	720
7	0	8	904	830
7	0	10	653	657
7	0	12	190	181
7	0	16	236	218
7	0	18	180	190
7	1	0	111	116
7	1	1	478	563
7	1	2	316	389
7	1	3	799	836
7	1	4	1433	1264
7	1	5	1306	1128
7	1	6	1449	1328
7	1	7	938	775
7	1	8	452	502
7	1	9	543	571
7	1	10	274	268
7	1	11	593	582
7	1	12	200	187
7	1	13	358	397
7	1	15	210	220
7	1	17	147	158
7	1	19	111	129
7	2	1	547	481
7	2	2	108	59
7	2	3	277	306
7	2	5	257	183
7	2	6	239	270
7	2	7	197	163
7	2	11	139	112
7	3	0	247	280
7	3	1	455	472
7	3	2	751	753
7	3	3	276	265
7	3	4	857	862
7	3	5	389	381
7	3	6	645	678
7	3	7	421	461
7	3	8	758	766
7	3	9	128	56
7	3	10	387	392
7	3	11	237	224
7	3	14	257	225
7	3	16	135	156
7	3	17	137	133

H	K	L	FOBS	FCALC
7	4	1	228	244
7	4	2	374	422
7	4	3	259	222
7	4	4	188	195
7	4	5	207	236
7	4	6	294	332
7	4	7	295	253
7	4	10	191	208
7	5	0	151	121
7	5	1	778	861
7	5	3	734	768
7	5	5	857	877
7	5	7	1020	1001
7	5	9	741	741
7	5	11	276	281
7	5	15	212	200
7	5	16	115	127
7	5	17	208	187
7	6	2	210	230
7	6	4	216	199
7	6	6	187	163
7	6	12	251	197
7	6	13	256	275
7	6	14	133	153
7	6	15	157	167
7	7	0	515	507
7	7	2	579	602
7	7	4	537	574
7	7	5	166	162
7	7	6	480	481
7	7	7	163	113
7	7	8	486	468
7	7	10	306	300
7	7	11	223	243
7	7	12	197	172
7	7	14	134	133
7	9	0	433	378
7	9	1	479	453
7	9	2	309	267
7	9	3	361	335
7	9	5	346	351
7	9	7	188	168
7	9	10	148	119
7	9	11	179	188
7	9	12	136	124
7	10	6	149	123
7	11	0	228	254

H	K	L	FOBS	FCALC
7	11	1	221	225
7	11	2	238	224
7	11	3	282	283
7	11	4	214	158
7	11	5	262	260
7	11	6	133	132
8	0	0	264	252
8	0	2	474	629
8	0	4	1507	1490
8	0	6	1304	1290
8	0	8	221	216
8	0	16	167	152
8	0	18	215	192
8	1	2	420	356
8	1	3	1023	864
8	1	5	780	761
8	1	6	366	318
8	1	7	275	206
8	1	8	378	356
8	1	9	530	481
8	1	10	309	291
8	1	11	286	293
8	1	12	157	136
8	1	13	158	162
8	1	15	255	206
8	1	16	190	196
8	1	18	223	211
8	2	0	161	157
8	2	1	443	449
8	2	2	301	271
8	2	3	952	870
8	2	5	1141	1120
8	2	7	852	813
8	2	8	201	170
8	2	9	483	464
8	2	10	170	184
8	2	11	280	253
8	2	13	143	141
8	2	17	120	83
8	3	3	334	313
8	3	5	391	393
8	3	6	516	526
8	3	7	223	198
8	3	8	212	183
8	3	10	264	255
8	4	0	506	516
8	4	1	806	827

H	K	L	FOBS	FCALC
8	4	2	612	629
8	4	3	342	289
8	4	4	584	529
8	4	5	194	187
8	4	6	483	476
8	4	7	346	331
8	4	8	433	436
8	4	9	300	302
8	4	10	138	120
8	4	14	250	219
8	4	16	224	199
8	5	1	125	161
8	5	2	145	179
8	5	3	132	130
8	5	5	315	302
8	5	7	540	534
8	5	8	164	193
8	5	9	248	270
8	5	11	287	287
8	5	13	400	382
8	5	15	229	245
8	6	0	198	201
8	6	2	319	354
8	6	4	296	315
8	6	5	317	317
8	6	6	357	331
8	6	7	414	382
8	6	8	494	518
8	6	9	352	346
8	6	10	276	285
8	6	11	156	168
8	7	5	148	187
8	7	10	215	199
8	7	12	195	182
8	7	14	193	214
8	8	1	490	513
8	8	3	318	318
8	8	4	200	210
8	8	5	331	355
8	8	6	200	197
8	8	7	213	207
8	8	9	169	152
8	8	11	222	240
8	8	13	116	107
8	9	2	205	204
8	9	7	188	201
8	10	0	154	151

10*FOBS & 10*FCALC FOR CR2[O2CNET2]4[NET2]2 (CHISHOLM, COTTON ET AL 1977)

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
8	10	2	201	215	9	4	15	166	195	10	1	11	272	284	10	7	2	155	151	11	3	2	256	282
8	10	4	293	277	9	4	16	218	222	10	1	12	151	200	10	7	4	207	224	11	3	4	232	223
8	10	6	225	244	9	5	3	165	200	10	1	13	245	269	10	7	6	194	143	11	3	5	285	220
8	10	8	209	202	9	5	7	271	241	10	1	14	146	138	10	7	8	180	199	11	3	8	148	175
9	0	2	354	366	9	5	8	138	122	10	1	15	289	305	10	7	10	239	259	11	3	9	141	125
9	0	4	190	122	9	5	9	167	173	10	1	16	188	188	10	7	12	274	224	11	4	2	147	83
9	0	8	784	753	9	6	2	197	186	10	1	17	303	302	10	8	3	147	159	11	4	4	374	362
9	0	10	965	960	9	6	4	329	343	10	2	0	351	362	10	8	5	189	188	11	4	5	148	180
9	0	12	586	581	9	6	5	265	251	10	2	1	184	151	10	8	7	147	159	11	4	6	384	383
9	0	14	380	375	9	6	6	335	328	10	2	3	244	246	10	8	9	124	128	11	4	7	203	211
9	0	16	317	340	9	6	7	397	416	10	2	4	243	218	10	8	10	129	128	11	4	8	168	180
9	0	18	337	310	9	6	8	157	151	10	2	5	291	248	10	9	3	279	295	11	4	11	202	177
9	1	0	142	113	9	6	9	322	315	10	2	6	286	253	10	9	5	195	199	11	4	12	199	183
9	1	1	252	251	9	6	10	186	205	10	2	8	212	232	10	9	9	134	138	11	4	13	168	187
9	1	3	523	473	9	6	11	198	180	10	2	14	165	128	10	10	0	157	195	11	4	14	190	185
9	1	5	570	499	9	6	12	301	281	10	3	2	169	103	10	10	2	137	147	11	4	15	156	165
9	1	6	143	107	9	6	13	169	195	10	3	3	157	168	11	0	2	123	189	11	4	16	175	152
9	1	8	291	262	9	6	14	241	238	10	3	5	149	193	11	0	4	536	455	11	5	0	125	97
9	1	9	178	130	9	6	15	160	152	10	3	6	225	208	11	0	6	400	403	11	5	1	503	533
9	1	10	216	223	9	7	1	146	115	10	3	7	306	350	11	0	8	359	354	11	5	3	614	610
9	2	1	185	183	9	7	4	218	278	10	3	8	170	99	11	0	10	359	303	11	5	5	407	440
9	2	2	320	315	9	7	6	370	359	10	3	9	152	136	11	0	12	237	217	11	5	7	267	289
9	2	3	208	203	9	7	8	158	151	10	3	12	199	252	11	0	14	200	208	11	5	8	146	137
9	2	4	354	329	9	8	9	132	90	10	3	14	385	379	11	0	16	326	305	11	5	9	316	300
9	2	5	450	450	9	8	11	156	146	10	3	16	292	303	11	1	0	332	333	11	5	11	229	233
9	2	7	236	200	9	9	4	255	245	10	3	17	141	139	11	1	1	614	611	11	5	13	154	171
9	2	9	379	345	9	9	5	164	201	10	4	1	281	269	11	1	3	705	692	11	5	14	115	94
9	2	11	200	180	9	9	6	200	207	10	4	2	128	113	11	1	4	327	273	11	5	15	114	105
9	2	15	205	185	9	9	7	176	199	10	4	4	309	279	11	1	5	222	211	11	6	2	137	116
9	2	17	295	295	9	9	9	197	182	10	4	8	386	369	11	1	6	635	575	11	6	3	160	171
9	3	0	1135	1090	9	10	2	140	147	10	4	10	189	186	11	1	7	207	212	11	6	5	171	172
9	3	2	820	757	9	10	4	200	213	10	4	14	126	146	11	1	8	320	308	11	6	6	155	104
9	3	3	220	182	10	0	0	291	189	10	5	2	152	207	11	1	9	244	220	11	6	9	136	30
9	3	4	491	471	10	0	2	113	145	10	5	4	181	197	11	1	10	171	189	11	6	13	138	117
9	3	6	517	502	10	0	4	384	356	10	5	5	238	215	11	1	13	224	249	11	6	14	143	142
9	3	8	374	375	10	0	6	769	803	10	5	7	375	390	11	1	15	162	182	11	7	0	293	298
9	3	9	163	163	10	0	8	408	460	10	5	11	250	203	11	2	1	289	308	11	7	1	137	118
9	3	10	175	161	10	0	14	269	262	10	5	13	359	363	11	2	3	261	239	11	7	2	216	249
9	3	11	185	192	10	0	16	197	216	10	5	15	277	292	11	2	4	123	77	11	7	4	144	151
9	3	13	155	156	10	1	1	156	102	10	6	0	184	188	11	2	7	191	224	11	7	8	201	194
9	4	1	218	210	10	1	2	148	94	10	6	1	139	127	11	2	9	188	159	11	7	10	174	162
9	4	2	193	203	10	1	4	397	359	10	6	2	193	217	11	2	11	229	262	11	7	11	164	166
9	4	6	347	376	10	1	6	145	168	10	6	3	232	236	11	2	13	436	421	11	7	12	144	140
9	4	8	185	178	10	1	7	165	180	10	6	8	162	168	11	2	14	149	161	11	8	3	170	211
9	4	12	210	243	10	1	8	259	289	10	6	10	299	300	11	2	15	338	352	11	8	5	154	162
9	4	13	290	297	10	1	9	333	303	10	6	12	159	190	11	2	17	219	254	11	8	6	150	135
9	4	14	325	314	10	1	10	490	455	10	7	1	137	116	11	3	0	273	304	11	8	8	144	121

10*FOBS & 10*FCALC FOR CR2[O2CNET2]4[NET2]2 (CHISHOLM, COTTON ET AL 1977) PAGE 6

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
11	8	9	180	159	12	4	12	256	263	13	3	2	730	728	14	1	1	183	260	15	0	4	191	242
11	8	11	168	173	12	4	14	149	169	13	3	4	504	485	14	1	2	173	224	15	0	12	196	197
11	9	0	186	198	12	5	5	166	205	13	3	5	162	158	14	1	3	255	270	15	0	14	302	270
11	9	1	186	177	12	6	0	579	622	13	3	6	219	226	14	1	10	182	209	15	1	0	279	282
11	9	2	132	111	12	6	1	158	139	13	3	8	292	295	14	1	12	176	173	15	1	1	184	198
12	0	0	1329	1468	12	6	2	406	391	13	3	9	147	144	14	1	14	126	124	15	1	3	190	163
12	0	2	1225	1297	12	6	3	376	396	13	3	10	319	316	14	1	15	159	137	15	1	7	179	156
12	0	4	675	707	12	6	4	388	404	13	3	11	319	321	14	2	1	723	751	15	1	9	261	245
12	0	6	467	470	12	6	5	324	302	13	3	12	241	254	14	2	2	304	312	15	1	12	146	147
12	0	8	611	587	12	6	6	421	447	13	3	13	134	153	14	2	3	534	535	15	1	13	122	114
12	0	10	400	364	12	6	7	243	269	13	3	14	217	215	14	2	4	203	228	15	2	1	147	107
12	0	12	180	174	12	6	8	162	168	13	4	7	199	200	14	2	5	273	256	15	2	5	164	130
12	1	1	127	139	12	6	9	234	228	13	4	14	144	128	14	2	7	260	247	15	2	9	174	198
12	1	2	320	316	12	6	10	170	193	13	5	1	567	586	14	2	8	207	199	15	2	11	233	252
12	1	3	251	257	12	6	11	145	150	13	5	2	178	155	14	2	9	426	439	15	2	13	148	184
12	1	4	171	145	12	6	12	210	190	13	5	3	554	548	14	2	11	382	405	15	3	0	295	329
12	1	7	138	166	12	6	13	178	191	13	5	5	474	468	14	2	13	216	227	15	3	1	298	307
12	2	0	364	388	12	8	1	312	330	13	5	7	293	265	14	3	4	145	174	15	3	2	277	278
12	2	1	598	618	12	8	3	225	235	13	5	9	236	257	14	3	7	144	139	15	3	3	219	208
12	2	2	387	378	12	8	7	133	139	13	5	11	257	271	14	3	12	126	108	15	3	4	368	364
12	2	3	458	473	12	8	8	126	156	13	5	13	198	202	14	4	0	402	424	15	3	6	451	439
12	2	5	671	647	12	8	9	200	210	13	6	7	148	173	14	4	1	172	169	15	3	8	329	354
12	2	7	319	328	12	8	10	139	147	13	6	9	131	144	14	4	2	365	335	15	3	10	280	317
12	2	8	139	95	12	10	2	178	194	13	7	0	336	338	14	4	3	189	194	15	3	12	229	224
12	2	13	230	255	13	0	2	654	659	13	7	1	177	244	14	4	4	414	372	15	4	1	134	107
12	2	14	120	131	13	0	4	257	195	13	7	2	388	378	14	4	5	296	346	15	4	2	267	264
12	2	15	170	184	13	0	10	306	288	13	7	3	148	103	14	4	6	367	383	15	4	7	209	208
12	3	1	201	201	13	1	0	736	792	13	7	4	331	338	14	4	7	246	243	15	4	8	143	113
12	3	2	132	133	13	1	1	755	734	13	7	5	177	128	14	4	8	246	235	15	4	9	230	227
12	3	3	371	387	13	1	2	526	551	13	7	6	288	317	14	4	10	244	217	15	4	10	146	155
12	3	4	163	177	13	1	3	592	619	13	7	8	320	317	14	4	11	183	165	15	4	11	171	134
12	3	5	276	288	13	1	4	224	200	13	7	10	189	208	14	4	12	147	166	15	4	12	185	180
12	3	6	270	297	13	1	5	450	472	13	8	9	116	110	14	4	13	159	147	15	5	1	206	177
12	3	8	266	233	13	1	6	135	121	13	9	1	150	178	14	5	11	194	199	15	5	5	132	94
12	3	10	212	195	13	1	7	418	407	13	9	2	129	111	14	6	0	206	221	15	5	9	118	76
12	3	12	287	293	13	1	8	165	191	13	9	3	170	174	14	6	1	364	378	15	6	8	143	117
12	3	13	133	133	13	1	9	244	260	13	9	4	134	154	14	6	2	254	269	15	6	10	176	183
12	3	14	259	279	13	1	10	246	258	13	9	5	203	194	14	6	3	234	269	15	7	0	257	265
12	4	0	487	420	13	1	11	181	194	13	9	6	168	172	14	6	4	288	278	15	7	2	245	273
12	4	1	419	377	13	1	12	230	210	14	0	0	709	672	14	6	9	142	124	15	7	4	173	179
12	4	2	446	429	13	1	13	158	162	14	0	2	504	472	14	7	7	132	122	16	0	0	261	277
12	4	3	441	409	13	1	14	117	102	14	0	4	215	211	14	7	8	129	136	16	0	6	235	236
12	4	4	320	354	13	2	3	222	230	14	0	6	253	253	14	7	10	109	103	16	1	4	156	156
12	4	6	154	149	13	2	5	297	269	14	0	8	289	270	14	8	1	250	271	16	1	5	170	147
12	4	8	227	224	13	2	11	146	118	14	0	10	256	265	14	8	3	247	250	16	1	6	156	145
12	4	9	215	232	13	3	0	685	710	14	0	12	343	335	14	8	5	289	312	16	1	7	174	130
12	4	10	383	392	13	3	1	182	211	14	0	14	186	166	14	8	7	266	284	16	1	9	143	147

10*FOBS & 10*FCALC FOR CR2[O2CNET2]4[NET2]2 (CHISHOLM, COTTON ET AL 1977)

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
16	1	11	151	136	18	0	8	148	173	20	2	1	312	336										
16	1	13	123	145	18	0	10	250	214	20	2	3	294	289										
16	2	1	144	137	18	1	5	142	106	20	2	5	300	296										
16	2	5	197	180	18	1	7	142	111	20	4	1	164	183										
16	2	6	134	110	18	1	9	145	142	20	4	2	142	170										
16	2	7	178	192	18	2	1	188	166	21	0	2	108	106										
16	3	2	163	130	18	2	5	156	175	21	1	1	127	110										
16	3	6	218	176	18	2	7	233	244	21	1	3	146	126										
16	3	8	292	288	18	2	8	128	122															
16	3	10	287	305	18	2	9	203	229															
16	3	11	143	149	18	3	8	178	171															
16	3	12	229	230	18	4	0	162	174															
16	4	0	160	211	18	4	2	209	219															
16	4	1	146	125	18	4	3	131	140															
16	4	3	145	119	18	4	4	170	193															
16	5	7	148	166	18	4	5	114	135															
16	5	9	192	184	18	4	6	131	122															
17	0	2	219	213	18	4	8	107	128															
17	0	4	204	149	18	6	0	110	100															
17	0	6	304	292	18	6	1	137	168															
17	0	8	191	221	18	6	3	167	182															
17	0	10	121	129	18	6	4	139	131															
17	1	0	256	267	19	0	2	183	214															
17	1	1	175	147	19	1	0	215	190															
17	1	3	161	167	19	1	1	183	183															
17	1	9	141	122	19	1	2	139	168															
17	1	11	122	70	19	1	3	140	135															
17	2	3	193	170	19	1	4	128	142															
17	2	7	175	181	19	1	5	231	183															
17	2	8	133	144	19	1	6	166	152															
17	2	9	211	195	19	1	7	191	181															
17	2	11	201	217	19	1	8	141	137															
17	3	0	137	143	19	1	9	160	159															
17	3	5	142	140	19	2	3	166	181															
17	3	10	106	66	19	3	0	178	172															
17	4	8	154	153	19	3	1	194	166															
17	4	10	187	219	19	3	2	262	264															
17	5	1	121	133	19	3	4	321	322															
17	5	3	192	191	19	3	6	279	295															
17	5	5	144	115	19	5	1	179	165															
17	5	7	124	118	19	5	3	195	220															
17	5	9	110	105	20	0	0	149	122															
17	7	4	137	111	20	0	2	168	149															
18	0	0	378	393	20	0	4	184	185															
18	0	2	242	241	20	0	6	210	198															
18	0	4	173	157	20	1	3	130	115															
18	0	6	185	198	20	1	4	113	140															

TECHNICAL REPORT DISTRIBUTION LIST

	No. Copies
Office of Naval Research Arlington, Virginia 22217 Attn: Code 472	2
Office of Naval Research Arlington, Virginia 22217 Attn: Code 102IP 1	6
ONR Branch Office 536 S. Clark Street Chicago, Illinois 60605 Attn: Dr. Jerry Smith	1
ONR Branch Office 715 Broadway New York, New York 10003 Attn: Scientific Dept.	1
ONR Branch Office 1030 East Green Street Pasadena, California 91106 Attn: Dr. R. J. Marcus	1
ONR Branch Office San Francisco Area Office One Hallidie Plaza San Francisco, Calif. 94102 Attn: Dr. Phillip A. Miller	1
ONR Branch Office 495 Summer Street Boston, Massachusetts 02210 Attn: Dr. L. H. Peebles	1
Director, Naval Research Laboratory Washington, D.C. 20390 Attn: Code 6100	1
The Asst. Secretary of the Navy (R&D) Department of the Navy Room 4E736, Pentagon Washington, D.C. 20350	1
Commander, Naval Air Systems Command Department of the Navy Washington, D.C. 20360 Attn: Code 310C (H. Rosenwasser)	1
Defense Documentation Center Building 5, Cameron Station Alexandria, Virginia 22314	12
U.S. Army Research Office P.O. Box 12211 Research Triangle Park, N.C. 27709 Attn: CRD-AA-IP	1
Naval Ocean Systems Center San Diego, California 92152 Attn: Mr. Joe McCartney	1
Naval Weapons Center China Lake, California 93555 Attn: Head, Chemistry Division	1
Naval Civil Engineering Laboratory Port Hueneme, California 93041 Attn: Mr. W. S. Haynes	1
Professor O. Heinz Department of Physics & Chemistry Naval Postgraduate School Monterey, California 93940	1
Dr. A. L. Slafkosky Scientific Advisor Commandant of the Marine Corps (Code RD-1) Washington, D.C. 20380	1
Office of Naval Research Arlington, Virginia 22217 Attn: Dr. Richard S. Miller	1

TECHNICAL REPORT DISTRIBUTION LIST

	No. Copies
Dr. M. A. El-Sayed University of California Department of Chemistry Los Angeles, California 90024	1
Dr. M. W. Windsor Washington State University Department of Chemistry Pullman, Washington 99163	1
Dr. E. R. Bernstein Colorado State University Department of Chemistry Fort Collins, Colorado 80521	1
Dr. C. A. Heller Naval Weapons Center Code 6059 China Lake, California 93555	1
~~Dr. M. H. Chisholm~~ ~~Princeton University~~ ~~Department of Chemistry~~ ~~Princeton, New Jersey 08540~~	1
Dr. J. R. MacDonald Naval Research Laboratory Chemistry Division Code 6110 Washington, D.C. 20375	1

	No. Copi
Dr. G. B. Schuster University of Illinois Chemistry Department Urbana, Illinois 61801	
Dr. E. M. Eyring University of Utah Department of Chemistry Salt Lake City, Utah	
Dr. A. Adamson University of Southern California Department of Chemistry Los Angeles, California 90007	
Dr. M. S. Wrighton Massachusetts Institute of Technolog Department of Chemistry Cambridge, Massachusetts 02139	
Dr. M. Rauhut American Cyanamid Company Chemical Research Division Bound Brook, New Jersey 08805	

TECHNICAL REPORT DISTRIBUTION LIST

	No. Copies
Dr. D. A. Vroom IRT P.O. Box 80817 San Diego, California 92138	1
Dr. G. A. Somorjai University of California Department of Chemistry Berkeley, California 94720	1
Dr. L. N. Jarvis Surface Chemistry Division 4555 Overlook Avenue, S.W. Washington, D.C. 20375	1
Dr. W. M. Risen, Jr. Brown University Department of Chemistry Providence, Rhode Island 02912	1
~~Dr. M. H. Chisholm~~ ~~Princeton University~~ ~~Chemistry Department~~ ~~Princeton, New Jersey 08540~~	1
Dr. J. B. Hudson Renssalaer Polytechnic Institute Materials Division Troy, New York 12181	1
Dr. John T. Yates National Bureau of Standards Department of Commerce Surface Chemistry Section Washington, D.C. 20234	1
Dr. Theodore E. Madey Department of Commerce National Bureau of Standards Surface Chemistry Section Washington, D.C. 20234	1
Dr. J. M. White University of Texas Department of Chemistry Austin, Texas 78712	1

	No. Copies
Dr. R. W. Vaughan California Institute of Technology Division of Chemistry & Chemical Engineering Pasadena, California 91125	1
Dr. Keith H. Johnson Massachusetts Institute of Technology Department of Metallurgy and Materials Science Cambridge, Massachusetts 02139	1
Dr. M. S. Wrighton Massachusetts Institute of Technology Department of Chemistry Cambridge, Massachusetts 02139	1
Dr. J. E. Demuth IBM Corp. Thomas J. Watson Research Center P.O. Box 218 Yorktown Heights, New York 10598	
Dr. C. P. Flynn University of Illinois Department of Physics Urbana, Illinois 61801	
Dr. W. Kohn University of California (San Diego) Department of Physics La Jolla, California 92037	
Dr. R. L. Park Director, Center of Materials Research University of Maryland College Park, Maryland 20742	

TECHNICAL REPORT DISTRIBUTION LIST

	No. Copies
Dr. W. T. Peria Electrical Engineering Department University of Minnesota Minneapolis, Minnesota 55455	1
Dr. Narkis Tzoar City University of New York Convent Avenue at 138th Street New York, New York 10031	1
Dr. Chia-wei Woo Northwestern University Department of Physics Evanston, Illinois 60201	1
Dr. D. C. Mattis Yeshiva University Physics Department Amsterdam Avenue & 185th Street New York, New York 10033	1
Dr. Robert M. Hexter University of Minnesota Department of Chemistry Minneapolis, Minnesota 55455	1
Dr. Leonard Wharton James Franck Institute Department of Chemistry 5640 Ellis Avenue Chicago, Illinois 60637	1
Dr. M. G. Lagally Department of Metallurgical and Mining Engineering University of Wisconsin Madison, Wisconsin 53706	1
Dr. Robert Gomer James Franck Institute Department of Chemistry 5640 Ellis Avenue Chicago, Illinois 60637	1
Dr. R. F. Wallis University of California (Irvine) Department of Physics Irvine, California 92664	1

TECHNICAL REPORT DISTRIBUTION LIST

	No. Copies
Dr. R. M. Grimes University of Virginia Department of Chemistry Charlottesville, Virginia 22901	1
Dr. M. Tsutsui Texas A&M University Department of Chemistry College Station, Texas 77843	1
Dr. C. Quicksall Georgetown University Department of Chemistry 37th & O Streets Washington, D.C. 20007	1
Dr. M. F. Hawthorne University of California Department of Chemistry Los Angeles, California 90024	1
Dr. D. B. Brown University of Vermont Department of Chemistry Burlington, Vermont 05401	1
Dr. W. B. Fox Naval Research Laboratory Chemistry Division Code 6130 Washington, D.C. 20375	1
Dr. J. Adcock University of Tennessee Department of Chemistry Knoxville, Tennessee 37916	1
Dr. A. Cowley University of Texas Department of Chemistry Austin, Texas 78712	1

	No. Copies
Dr. W. Hatfield University of North Carolina Department of Chemistry Chapel Hill, North Carolina 27514	1
Dr. D. Seyferth Massachusetts Institute of Technology Department of Chemistry Cambridge, Massachusetts 02139	1
~~Dr. M. H. Chisholm~~ ~~Princeton University~~ ~~Department of Chemistry~~ ~~Princeton, New Jersey 08540~~	1
Dr. B. Foxman Brandeis University Department of Chemistry Waltham, Massachusetts 02154	1
Dr. T. Marks Northwestern University Department of Chemistry Evanston, Illinois 60201	1
Dr. G. Geoffrey Pennsylvania State University Department of Chemistry University Park, Pennsylvania 16802	1
Dr. J. Zuckerman University of Oklahoma Department of Chemistry Norman, Oklahoma 73019	1